The Fourth
AICS International Symposium

Computer and Computational Sciences for Exascale Computing

December 2—3, 2013, Kobe, JAPAN

Organized and Sponsored by RIKEN AICS

This Symposium is a part of RIKEN Symposium Series.

Supported by:

RIKEN HPCI Program for Computational Life Sciences
Computational Materials Science Initiative
JAMSTEC: Japan Agency for Marine-Earth Science and Technology
Institute of Industrial Science, the University of Tokyo
Japan Atomic Energy Agency
Japan Aerospace Exploration Agency
Joint Institute for Computational Fundamental Science (JICFuS)
Information Initiative Center, Hokkaido University
Cyberscience Center, Tohoku University
Center for Computational Sciences, University of Tsukuba
Information Technology Center, the University of Tokyo
Global Scientific Information and Computing Center, Tokyo Institute of Technology
Information Technology Center, Nagoya University
Academic Center for Computing and Media Studies, Kyoto University
Cybermedia Center, Osaka University
Research Institute for Information Technology, Kyushu University
National Institute of Informatics

The Fourth
AICS International Symposium

Computer and Computational Sciences for Exascale Computing

Invited Lecture Program

December 2 (Monday)

Opening Remarks

09:30 – 09:45 Kimihiko Hirao
(RIKEN Advanced Institute for Computational Science)

HPC in Computational Disaster Mitigation and Reduction

09:45 – 10:25 **Seismic damage simulation of buildings in urban areas based on GPU and a physics engine**
Xinzheng Lu 10
(Department of Civil Engineering, Tsinghua University)

10:25 – 10:55 **Application of high performance computing to seismic structure response analysis**
Muneo Hori 11
(RIKEN Advanced Institute for Computational Science)

Break

10:55 – 11:10

HPC in Discrete Event Simulation

11:10 – 11:50 **Computational Sociology: Study of Social Networks**
Kimmo Kaski 12
(Department of Biomedical Engineering and Computational Science, Aalto University, Finland)

11:50 – 12:20 **From people to society, a supercomputer challenge**
Nobuyasu Ito 13
(RIKEN Advanced Institute for Computational Science)

Lunch and Poster Session

12:20 – 14:00

Future HPC Session 1

14:00 – 15:00 **Creating a Gentle Slope to Yottaflop Computations: the Global View Resilience (GVR) Project**
Andrew Chien 14
(University of Chicago)

15:00 – 15:15 **Brief Introduction of HPC Usability Research Team**
Toshiyuki Maeda 15
(RIKEN Advanced Institute for Computational Science)

15:15 – 15:30 **Technology Infrastructure for Scientific Applications with Large-Scale Dataset**
Kenji Ono 16
(RIKEN Advanced Institute for Computational Science)

15:30 – 15:45 **Research Activities in AICS towards post Peta-scale Numerical Libraries**
Toshiyuki Imamura 17
(RIKEN Advanced Institute for Computational Science)

Break
15:45 – 16:00

16:00 – 17:00 **The Mont-Blanc project: Are mobile processors ready for HPC?**
Paul Carpenter 18
(Barcelona Supercomputing Center)

Banquet
17:30 – 19:30 (Optional)

December 3 (Tuesday)

HPC in Computational Structural Biology

09:30 – 10:10 **Large-scale simulations of molecular machines: quantifying the energy landscape of the ribosome**
Karissa Sanbonmatsu 21
(Theoretical Biology and Biophysics, Theoretical Division, Los Alamos National Laboratory)

10:10 – 10:40 **Structural modeling of biological molecules from low resolution experimental data**
Florence Tama 22
(RIKEN Advanced Institute for Computational Science)

Break
10:40 – 11:00

HPC in Computational Chemistry

11:00 – 11:40 **The allosteric communication pathways in KIX domain of CBP**
Michele Parrinello 23
(Department of Chemistry and Applied Biosciences, ETH Zurich, and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, Lugano)

11:40 – 12:10 **Recent Advances in LC-DFT**
Kimihiko Hirao 24
(RIKEN Advanced Institute for Computational Science)

Lunch and AICS Tour

12:10 – 14:00

Future HPC Session 2

14:00 – 15:00 **Blue Waters and the Future of @Scale Computing and Analysis**
Bill Kramer 25
(National Center for Supercomputing Applications)

15:00 – 15:15 **NTChem and Beyond**
Michio Katouda 26
(RIKEN Advanced Institute for Computational Science)

15:15 – 15:30 **Elementary Particle Physics in Future HPC**
Yoshinobu Kuramashi 27
(RIKEN Advanced Institute for Computational Science)

15:30 – 15:45 **Large Scale Numerical Simulations for Strongly Correlated Quantum Systems: Density Matrix Renormalization Group in Two-Dimensions**
Seiji Yunoki 28
(RIKEN Advanced Institute for Computational Science)

Break

15:45 – 16:00

16:00 – 16:25 **Report on Feasibility Study on Future HPC Infrastructure – Approach from General Purpose CPU Architecture –**
Yutaka Ishikawa 29
(RIKEN Advanced Institute for Computational Science)

16:25 – 16:50 **Report on Feasibility Study on Future HPC Infrastructure – Toward Exascale Accelerated Computing –**
Mitsuhisa Sato 30
(RIKEN Advanced Institute for Computational Science)

16:50 – 17:15 **Future social and scientific subjects resolved by science-driven HPC**
Hirofumi Tomita 31
(RIKEN Advanced Institute for Computational Science)

Closing Remarks

17:15 – 17:30 Akinori Yonezawa
(RIKEN Advanced Institute for Computational Science)

Poster Session Program

Invited Lecture

December 2 (Monday)

Speakers List

Xinzheng Lu

Muneo Hori

Kimmo Kaski

Nobuyasu Ito

Andrew Chien

Toshiyuki Maeda

Kenji Ono

Toshiyuki Imamura

Paul Carpenter

Seismic damage simulation of buildings in urban areas based on GPU and a physics engine

Xinzheng Lu. Zhen Xu, Bo Han, Chen Xiong
Key Laboratory of Civil Engineering Safety and Durability of China Education Ministry, Department of Civil Engineering, Tsinghua University, Beijing 100084, P.R. China.

Seismic damage simulation of buildings is an important task in improving earthquake resistance and safety of dense urban areas. There are two critical technical challenges for such a simulation: high-performance computing and realistic display. To overcome the computing bottleneck due to a large number of buildings, a high-performance computing approach based on graphics processing unit (GPU) is proposed. The benchmark cases demonstrate the performance-to-price ratio of the proposed approach can be 39 times as great as that of a traditional central processing unit (CPU) approach. To realistically display seismic damage, a simplified simulation algorithm of building collapse is proposed based on physics engine. Due to its significant advantages on multi-body dynamics and collision detection, physics engine can efficiently simulate complex movement and interactive collisions in the process of building collapse. Finally, a seismic damage simulation of a medium-sized urban area is implemented to demonstrate the capacity and advantages of the proposed methods.

Application of high performance computing to seismic structure response analysis

Muneo Hori
RIKEN AICS

Local and overall collapse analysis is a key element in evaluating the seismic performance of reinforced concrete structures, but analysis of multiple cracking which takes in concrete has been a bottleneck of this simulation. High performance computing enables us to construct a high fidelity model of a target reinforced structure and analyze initiation and propagation processes of multiple cracking. An efficient solver which is based on a conjugate gradient method is used to achieve high numerical efficiency for a model whose degree-of-freedom exceeds hundred times larger than that of an ordinary model. A new discretization scheme, called particle discretization scheme (PDS), is developed to further enhance the multiple cracking analysis. It is easy to implement PDS into FEM, and the resulting PDS-FEM is able to determine complicated crack surface configuration, without introducing any new degree-of-freedom. The applicability of high performance computing to the seismic structure response analysis is demonstrated. Presented are three examples of PDS-FEM analysis, namely, a shear connector, a connector of steel segment and a set of piers for high ways. It is shown that the processes of initiation and propagation of multiple cracking are computed by PDS-FEM, and that the cracking pattern is in agreement with the experimental observations.

Computational Sociology: Study of Social Networks

Kimmo Kaski
Department of Biomedical Engineering and Computational Science,
Aalto University School of Science, Finland

Over the past decade Network Theory combined with Computational Science approach has turned out to be a powerful methodology to investigate complex systems of various sorts. Through computational data analysis, modeling, and simulation quite an unparalleled insight into the structure, function, and response of these systems can be obtained. In human societies individuals are linked through social interactions, which today takes place increasingly electronically due to Information Communication Technology thus leaving "footprints" of human behaviour recorded digitally as ever-increasing datasets. For the studies of these datasets the network theory and computational approach is a natural one as we have demonstrated by analysing the records of multi-million user mobile phone communication-logs. This social network turned out to be modular in structure showing communities within which individuals are connected with stronger ties and between communities they are connected with weaker ties. In addition we found the network topology and the weighted links for pairs of individuals to be related. These empirical findings inspired us to take the next step in network theory, namely developing a simple model based on network sociology mechanisms for making friends, in order to catch some salient features of meso-scale community and macro-scale topology formation. Our model turned out to produce many empirically observed features of large-scale social networks. In addition to the above-described structural analysis of human social networks we have also investigated the dynamics of social interaction. This is done by including into the data analysis demographic data, i.e. gender and age information of the individual mobile phone service subscriber. In this way we are able to look at the patterns of social behaviour and changes therein for individuals of different gender and age. To summarize we believe that the network theory approach to social systems combined with computational data analysis, modeling, and simulation, which we call Computational Sociology, can open up a new and quantitative perspective for studying and even predicting collective social phenomena such as information spreading, formation of societal structures, and evolutionary processes in them.

From people to society, a supercomputer challenge

Nobuyasu Ito
Discrete-event simulation research tesm, RIKEN AICS

Human society have been co-evolving with information and communication technologies since the beginning of our history. This co-evolution was accelerated with modern sciences and engineering, and especially computers and global information networks are boosting it up the more intimate and tangled stage. Now big-data mining and agent-based modeling for social phenomena are popular and handy applications of computers. But our society consists of complex subsystems, and it is characterized by well-balanced variety and diversity. Naive models of whole society comprise enormous number of sensitive parameters, and ways toward well-posed modeling are meandering around forests of combinatorial complexity.

Two challenges to such diversity and complexity are introduced in this presentation: a mass-execution and administration software named *OACIS*, and a model of diversity. The former is to tame rough behavior of models, and the latter will be a guiding light in complexity.

Creating a Gentle Slope to Yottaflop Computations

the Global View Resilience (GVR) Project

http://gvr.cs.uchicago.edu/
Andrew A. Chien
William Eckardt Professor in Computer Science
The University of Chicago and Argonne National Laboratory

The advent of submicron transistor scaling, power limits, and million-node machines give rise to new reliability challenges for exaflop (10^18 flops/sec) systems, and yottaflop (10^24 flops) computations. We believe that meeting these challenges will require application investment, sofware-hardware partnership, and aggressive hardware engineering. The goal of the GVR project is to enable applications to meet these challenges in a portable, flexible fashion.

We will describe the philosophy and design of the Global ViewResilience (GVR) project. First, the GVR system enables applications to describe error detection and recovery based on portable, high-level semantics. To achieve this, GVR employs a portable data abstraction, multi-version arrays, so the investment is preserved across machines. The use of multi-version enables robust recovery, even to "silent" or "latent" errors. Second, the GVR system enables cross-layer software-hardware partnership in detecting and recovering from errors, increasing the variety of errors that can be gracefully corrected. The key element to achieve this is a unified signalling and recovery interface which enables information, decision making, and recovery to be distributed across layers.

We will describe early results involving application experiments with the GVR system, exploring API design, error checking and handling, and impact.

Brief Introduction of HPC Usability Research Team

Toshiyuki Maeda
RIKEN Advanced Institute for Computational Science (AICS)

Today, computing (or computer simulation) is considered as an inevitable method for science, which is as important as theoretical and experimental studies. To conduct sufficiently precise and large-scale computer simulations for developing new scientific knowledge and insight, it sometime requires huge amount of computing resources. Thus, the importance of high performance computing (HPC) is increasing rapidly. Not only in academia, but also in industry, the role of HPC is expanding (for example, in the fields of drug discovery, financial applications, and so on).

Unfortunately, however, because conventional HPC requires special skills (especially in parallel, concurrent, and/or distributed programming), the growth of numbers of users and developers seems to be relatively weak, compared to, for example, web based applications, smartphone applications, cloud computing, and so forth. Thus, it results in a less innovative environment from the viewpoint of computer (information) science and technology.

The mission of HPC Usability Research Team is to research and develop a framework for liberating large-scale HPC to wide-range of users and developers. This talk gives a brief introduction and progress report about our ongoing research topics. More specifically, computing portal technologies for lowering the threshold of using and developing computing services, virtualization technologies for achieving security and fairness among multiple users and developers, software verification approaches for helping developers to find problems in their programs, evidence-based performance tuning technology, and so forth are explained, as much as time allows.

Technology Infrastructure for Scientific Applications with Large-Scale Dataset

Kenji Ono
Advanced visualization research team, RIKEN AICS

One purpose of our research is to discover useful knowledge from data obtained from scientific or engineering simulation and to return research results to society by applying derived findings. High-performance applications use plenty of processors and generate large number of files, especially in case of time-varying calculation. The large number of generated files prevent us from efficient execution of an analysis process. Usually, an analysis process consists of several tasks such as a model generation, simulation, data analysis, visualization and automation processing. Files are conventionally used as a way of connecting tasks to each other, however, the existence of large and numerous files becomes a bottleneck. Therefore, file handling is one of the important key technologies in large-scale parallel computation. So far, many studies have been done in the field of high-performance storage. In this talk, I will present how to organize and treat a bunch of distributed files with respect to a real application. Furthermore, I will show the design policy of using metadata to manage distributed files.

Another important key technology for handling a large-scale dataset is data compression. The challenge is to develop parallel algorithm to compress data. The simulated files are compressed using POD, an algorithm that can effectively compress source data in recursive order, and can be implemented using fast eigenvalue calculation. The particular POD algorithm we have created is accelerated by an efficient parallel load balancing method called a 2-3-4 combination partitioning and it works for any number of files. Then, compressed dataset is visualized by a large-scale visualization system operated on the K computer. A renderer based on ray tracing enables us to depict images efficiently using all and every nodes.

Research Activities in AICS towards post Peta-scale Numerical Libraries

Toshiyuki Imamura
RIKEN Advanced Institute for Computational Science

Abstract

As high-performance numerical libraries are of significance for the development of large-scale scientific simulation codes, our team mission is quite important towards the post peta scale supercomputer system. We should consider non homogeneous hardware configuration with many-core processors, accelerator processing units, and etc. The system software must have a layered structure in execution model as well as the hardware structure. Offloading the user programs, numerical libraries, and particular system routine will become more complicated. How to conceal such a complex structure and difficulties in programming or how to simplify the treatment of all the issues from software to hardware are the present theme in our study. Higher level abstraction may be one of the key issues for them. Highly parallelism', 'high performance', 'high precision', 'resiliency', and 'scalability' are also big issues.

In this talk, several reviews on numerical libraries of the K supercomputer system. The outline of our mission towards post peta-scale supercomputer system will be presented.

Keywords

K computer, KMATHLIB, post Peta-scale computer, Numerical library, Parallel algorithm

The Mont-Blanc project: Are mobile processors ready for HPC?

Paul M. Carpenter
Barcelona Supercomputing Center

In the late 1990s, there was a dramatic shift in high-performance computing, as special-purpose vector and SIMD machines were displaced by clusters of commodity desktop microprocessors. Microprocessors were considerably slower than special-purpose processors and their use required a change in programming model, but, once their floating-point performance reached about one tenth that of the incumbent technology, their adoption became inevitable, given that they were 50 times cheaper. This strong cost advantage led to a transformation so effective that the TOP500 list is still dominated by the x86 architecture.

In 2013, the largest commodity market in computing is not PCs or servers, but mobile computing, comprising smartphones and tablets, most of which are built with ARM-based SoCs. Mobile SoCs now have integrated floating-point units, making them capable of HPC, and they enjoy a similar cost advantage over server processors. We may therefore be about to see another step in the evolution of HPC, in which a new class of commodity processor replaces the incumbent technology due to its cost efficiency.

At the Barcelona Supercomputing Center, we are evaluating the performance and energy-efficiency of clusters of mobile SoCs, through our series of ARM-based prototypes. This talk will describe our work so far, and present our results, lessons learnt, and roadmap for the future. In summary, we give our view as to whether mobile SoCs are ready for HPC.

Invited Lecture

December 3 (Tuesday)

Speakers List

Karissa Sanbonmatsu

Florence Tama

Michele Parrinello

Kimihiko Hirao

Bill Kramer

Takahito Nakajima

Yoshinobu Kuramashi

Seiji Yunoki

Yutaka Ishikawa

Mitsuhisa Sato

Hirofumi Tomita

Large-scale simulations of molecular machines: quantifying the energy landscape of the ribosome

Karissa Sanbonmatsu
Theoretical Biology and Biophysics, Theoretical Division, Los Alamos National Laboratory

The ribosome is the universal molecular machine responsible for implementing the genetic code in all organisms. Specifically, the ribosome reads genetic information encoded in messenger RNA and assembles corresponding proteins. In a process called translocation, the ribosome must move by exactly three nucleotides along the mRNA in a processive fashion. This process entails large-scale, global conformational changes of the ribosome complex, accompanied by local conformational changes of its many parts. As opposed to a lock-step movement of the ribosome and its parts, a new picture has emerged: fluctuations of these parts occur stochastically and at different time scales. Energy landscapes can be used to characterize this complex picture. Here, translocation can be described as a series of transitions between energetic basins, where each basin represents a stable configuration (e.g., classical) and the fluctuations around this configuration. We use large-scale molecular dynamics simulations in combination with kinetic data to estimate barrier heights in the energy landscape. In addition, we explore the various conformational changes occurring during translocation and comment on their implications for translocation of mammalian ribosomes.

Structural modeling of biological molecules from low resolution experimental data

Florence Tama
RIKEN Advanced Institute for Computational Science

Cryo Electron Microscopy (cryo-EM) has become an essential tool for structural biology research. With recent progresses in experiments and new computer resources available, it is critical to continue to improve and develop computational tools to integrate cryo-EM with other experiments (X-ray, NMR) and extract information about structure and dynamics of biological molecules. In particular, as the number of structures deposited in the Protein Data Bank (PDB) by fitting a high-resolution structure into a low-resolution cryo-EM map is increasing, there is a need to revise the protocols and improve the measures for fitting. We will discuss methods we have developed to that effect as well as some of the applications of these approaches to study function of biological molecules. Finally we will also discuss our recent efforts to analyze X-ray Free Electron Laser (XFEL) data.

The allosteric communication pathways in KIX domain of CBP

Prof. Michele Parrinello
Department of Chemistry and Applied Biosciences, ETH Zurich, and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, Via G. Buffi 13, 6900 Lugano, Switzerland

Allosteric regulation plays an important role in a myriad of biomacromolecular processes. Specifically, in a protein, the process of allostery refers to the transmission of a local perturbation, such as ligand binding, to a distant site. Decades after the discovery of this phenomenon, models built on static images of proteins are being reconsidered with the knowledge that protein dynamics plays an important role in its function. Molecular dynamics simulations are a valuable tool for studying complex biomolecular systems, providing an atomistic description of their structure and dynamics. Unfortunately, their predictive power has been limited by the complexity of the biomolecule free-energy surface and by the length of the allosteric timescale (in the order of milliseconds). In this work, we are able to probe the origins of the allosteric changes that transcription factor mixed lineage leukemia (MLL) causes to the interactions of KIX domain of CREB-binding protein (CBP) with phosphorylated kinase inducible domain (pKID), by combing all-atom molecular dynamics with enhanced sampling methods recently developed in our group. We discuss our results in relation to previous NMR studies. We also develop a general simulations protocol to study allosteric phenomena and many other biological processes that occur in the micro/milliseconds timescale.

Recent Advances in LC-DFT

Kimihiko Hirao
Advanced Institute for Computational Science, RIKEN, Kobe, Japan

Density functional theory (DFT) has emerged as a powerful computational tool for molecular systems. The most appealing features of DFT are that everything is obtained directly from an observable and we are led to a one-particle Kohn-Sham (KS) theory. It is simple and conceptual. KS-DFT calculation takes about the same amount of time as Hartree-Fock (HF) calculation, yet unlike HF, we get a correlated result from KS-DFT.

Many of the problems of KS-DFT have mostly been a consequence of not having accurate functionals and potentials. Recently there has been considerable interest in our long-range correction (LC) DFT. In the LC scheme the exchange functional is partitioned with respect to the inter-electronic separation into long-range and short-range parts using a standard error function.

Accurate results can be obtained with such LC partitioning in terms of the reproduction of atomization energies, barrier heights, reaction enthalpies, geometrical properties, excitation energies (including CT and core excitations) and corresponding oscillator strengths over a wide range of molecular systems. Moreover, LC successfully provides a good description of linear and nonlinear polarizabilities of long-chain molecules and weak van der Waals interactions.

Recently it was demonstrated that the LC satisfies Koopmans' theorem, which implies that the eigenvalues and eigenvectors connected to the LC Kohn-Sham equation have a strict physical meaning.

Recent progress of LC-DFT will be presented.

Blue Waters and the Future of @Scale Computing and Analysis

William Kramer
National Center for Supercomputing Applications/University of Illinois Urbana-Champaign

Blue Waters is one of the premier extreme scale computational and data analysis resources in the world. This talk explores the important challenges the Blue Waters Sustained Petascale system is addressing and how the experience of supporting some of the most intense and scalable applications in the world can guide the design of future systems. Further lessons include the benefits and challenges of topology and heterogeneity.

NTChem and Beyond

RIKEN AICS Computational Molecular Science Research Team

An atomic- and molecular-level understanding of drug actions and the mechanisms of a variety of chemical reactions will provide insight for developing new drugs and materials. Although a number of diverse experimental methods have been developed, it still remains difficult to investigate the state of complex molecules and to follow chemical reactions in detail. Therefore, a theoretical molecular science that can predict the properties and functions of matter at the atomic and molecular levels by means of molecular theoretical calculations is keenly awaited as a replacement for experiment. Theoretical molecular science has recently made great strides due to progress in molecular theory and computer development. However, it is still unsatisfactory for practical applications. Consequently, our main goal is to realize an updated theoretical molecular science by developing a molecular theory and calculation methods to handle large complex molecules with high precision under a variety of conditions.

To achieve our aim, we have so far developed several methods of calculation. Examples include a way for resolving a significant problem facing conventional methods of calculation, in which the calculation volume increases dramatically when dealing with larger molecules; a way for improving the precision of calculations in molecular simulations; and a way for high-precision calculation of the properties of molecules containing heavy atoms such as metal atoms. We have integrated these calculation methods into a software package named NTChem that we are developing, which can run on the K computer and which contains a variety of high-performance calculation methods and functions. By selecting and combining appropriate methods, researchers can perform calculations suitable for their purpose. For example, it is possible to obtain a rough prediction of the properties of a molecule in a short period of time, or obtain a precise prediction by selecting a longer simulation. In addition, NTChem is designed for high performance on a computer with many compute nodes (high concurrency), and so it makes optimum use of the K computer's processing power.

In this talk, we will introduce the current and future projects for the NTChem software.

Elementary Particle Physics in Future HPC

Yoshinobu Kuramashi
University of Tsukuba/RIKEN AICS

After a brief review of scientific target in elementary particle physics in future HPC, we explain expected key algorithms and computational techniques and discuss possible difficulties associated with specific features of future computer architecture.

Large Scale Numerical Simulations for Strongly Correlated Quantum Systems: Density Matrix Renormalization Group in Two-Dimensions

Seiji Yunoki
Computational Materials Science Research Team, RIKEN AICS, Kobe, Japan

One of the most wealth fields in condensed matter physics is a kind of strongly correlated quantum systems where many-body interactions dominate determining fundamental physical properties. These systems include Hubbard-like models and frustrated quantum spin models, which are relevant, for example, to high-T_c cuprate superconductors and quantum spin liquids, respectively. The widely accepted consensus is that there is no ultimate numerical method at the present to solve a reasonably wide range of strongly correlated quantum systems in spatial dimensions higher than one-dimension (1D). In this talk, I will discuss our recent progress in numerically exactly solving strongly correlated quantum systems in two dimensions (2D) using density matrix renormalization group (DMRG) method. It is well known that DMRG method is superior in treating 1D systems as well as quasi-1D systems while in 2D its advantage is limited since, according to the area low of the entanglement entropy, the number of lowest eigenstates kept of the density matrix increases exponentially. To overcome this difficulty, here we introduce a real space parallelization scheme where a number M of DMRG sweeps can be done independently in separate processes, thus highly suitable to massively parallel computers such as K computer. This enables us to reach must fast convergence of the calculation with a fixed M and therefore we can focus only on increasing M to gain desirable numerical accuracy, which can be also treated effectively in passively parallel computers. We demonstrate this scheme by taking a 2D quantum spin S=1/2 system and discuss the efficiency comparing the conventional 2D DMRG scheme.

Report on Feasibility Study on Future HPC Infrastructure
--- Approach from General Purpose CPU Architecture ---

Yutaka Ishikawa
RIKEN AICS/ University of Tokyo

The University of Tokyo, Kyushu University, Fujitsu, Hitachi, and NEC in cooperation with RIKEN AICS have been studying a future supercomputer system towards an exascale supercomputer. It is assumed that the first target system will be deployed around 2018 with up to 30 MW and 2000 m^2 constraints. The purpose of this project is to design such a system and reveal what kind of researches and developments must be taken into account. Based on the K computer architecture, a new architecture has been designed and evaluated to cover a wide range of applications. At the same time, the system software stack for both the new architecture and commodity-based machines has been designed in order to assure general versatility. A prototype system software is being implemented using Xeon and Xeon phi processors. In the prototype system, a light-weight micro kernel, called McKernel, runs on cores for applications and Linux kernel runs on cores for OS services. On top of Linux and McKernel, a low level communication layer is being design in order to hide the communication hardware layer and provide remote-DMA-based scalable low-latency communication library. A parallel file I/O facility, an MPI communication library, parallel programming languages will be implemented using this low level communication layer. In this talk, after describing an overview of this study, the system software, designed and implemented in this study, is introduced.

Report on Feasibility Study on Future HPC Infrastructure
--- Toward Exascale Accelerated Computing ---

Mitsuhisa Sato
RIKEN AICS/ University of Tsukuba

The US, Europe, Japan and China are racing to develop the next generation of supercomputer – exascale machines - capable of a million trillion calculations a second by around 2020. To realize exascale systems, there are many challenges and issues including the limitation of power consumption and architectures to realize strong-scaling. One of promising approaches is an accelerated computing which uses specialized hardware, such as GPU, to speed up certain computational tasks, offering users energy efficiency, high performance for strong scaling.

Toward a post-petascale system as the next of Japan's petascale facility, the K computer, we, the group of the University of Tsukuba, Tokyo Institute of Technology, Aizu University, and RIKEN AICS have been carrying out a “Feasibility Study" project to study future supercomputer system towards an exascale supercomputer. We focus on the technology of accelerated computing for the extreme power-performance efficiency and the enabling technology for strong scaling of parallel scientific applications. As a result of our study, we are proposing the extreme SIMD architecture called PACS-G. This architecture are designed in the process of co-design with architectures, programming models and applications for the accelerated exascale computing.

In this talk, some issues and technologies of accelerated computing for exascale systems will be addressed, and the overview and current status of our project will be presented as well as some perspectives for post-petascale systems in Japan.

Future social and scientific subjects resolved by science-driven HPC

Hirofumi TOMITA
RIKEN / Advanced Institute for Computational Science

HPCI (High Performance Computing Infrastructure) Feasibility Study from the application community has started since July 2012. In this study, we have been discussing what and how the computational sciences do contribute to the general public and each of science fields by using the future HPCI. We investigate the possibility of HPC use not only in the existing major fields (life science, material science, earth science, manufacturing, fundamental physics) but also in new disciplines, e.g., social science. One of the most important conclusions is that the cooperation of multi-disciplines is necessary for resolving the social problems that we are now facing to.

In order to clarify the perspective for resolving them, we reorganize subjects extracted in this study into the following categories, which should be tackled over the traditional disciplines: drug design and health care, disaster prevention, energy and environment problem, and social science. Of course, conventional disciplines, which have been sophisticated so far in each of science areas, also should be enhanced to get comprehensive knowledge by understanding of nature. New scientific progress by cooperation with each discipline and big experimental facilities (e.g., particle accelerator, satellite, and so on) is also important.

There are various application programs to resolve such subjects. In order to estimate proposed future-systems systematically, we have started to prepare a set of "mini-applications", which is constructed from full applications, considering their practical use.

Poster Session

December 2 (Monday)

1P

An Implementation of Pseudo-Potential in a quantum chemical program based on Multi-wavelet Basis set

S. Yamada[1], H. Sekino[1*]

[1]Department of Computer Science and Engineering, Toyohashi University of Technology, 1-1 Hibarigaoka Toyohashi, 441-8580, Japan

*E-mail: sekino@tut.jp; +81-(0)532-44-6880

Key words: Pseudo-Potential, MRMW, MADNESS.

Recently, the progress of hardware and software made the first principle quantum chemical computation of large molecules possible in reasonable time. However, further improvement of accuracy and reduction of computational cost are desirable for applications to important bio-and nano-scale molecular systems.

Pseudo-Potential(PP) drastically reduces a computational cost especially for heavy elements. It is a method to reduce the amount of calculational cost by replacing inner shell electrons with local and non-local potentials(Fig.1). The local part $V^{loc}(r)$ of PP is given by[1)]

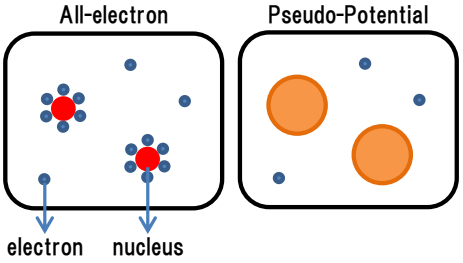


Fig.1 All-electron and Pseudo-Potential:

$$V^{loc}(r) = -\frac{Z_{ion}}{r}\,\mathrm{erf}\left(\frac{r}{\sqrt{2}r_{loc}}\right) + exp\left[-\frac{1}{2}\left(\frac{r}{r_{loc}}\right)^2\right]\sum_i C_i\left(\frac{r}{r_{loc}}\right)^{2i}$$

where erf denotes the error function. Z_{ion} is the ionic charge, and r_{loc} gives the range of the Gaussian ionic charge distribution leading to the erf potential.

The non-local part is given by[1)]

$$V^{nloc}(r) = \sum_l \sum_{i=1}^{3}\sum_{j=1}^{3}\sum_m |Y_{l,m}p_i^l\rangle\, h_{i,j}^l \langle Y_{l,m}p_j^l|$$

$$p_i^l(r) = N_{l,i}\left(\frac{r}{r_l}\right)^{l+2(i-1)} \exp\left[-\frac{1}{2}\left(\frac{r}{r_l}\right)^2\right], \int p_i^l(r)\, p_i^l(r) r^2 dr = 1$$

where $Y_{l,m}$ denotes a spherical Harmonic.

MADNESS[2)] is a scientific calculation library that targets massively parallel computing and using MRMW(multi-Resolution Multi-Wavelet) basis that is constructed based on Discrete Wavelet Transform technique. We implement the PP and compare the orbital energy computed with the PP, against the one without PP in MADNESS for Li, Be, LiH (Table 1). We show the results in Table1 and conclude that the result for the s-orbital is correct.

Table 1 Result of compared orbital energy

Target		Orbital energy[a.u.] All-electron	Pseudo-Potential	Error
Li	2s	-0.11633	-0.11755	0.00122
Be	2s	-0.20574	-0.20572	0.00002
LiH	2s	-0.16111	-0.16109	0.00003

References

1) S.Goedecker, M.Teter, and J.Hutter. Physical Review B 58(7), 3641-3662, (1996)
2) <http://www.csm.ornl.gov/ccsg/html/projects/madness.html>(2013/8/30)

2P

Dynamic load balance for a granular simulation using billion particles on GPU supercomputer

Satori Tsuzuki† Takayuki Aoki†

†Tokyo Institute of Technology

Distinct Element Method (DEM) is used for numerical simulations of granular mechanics. Particles interact with near particles by contact forces in both the normal and the tangential directions. To bring the simulation closer to the real phenomena, it is necessary to execute large-scale DEM simulations on modern high-performance supercomputers.

We have developed a DEM simulation code for a supercomputer with a large number of GPUs. Domain decomposition is a reasonable way for the DEM numerical algorithm. However, in the static domain decomposition, the particle distribution changes in time and space and the computational load for each domain becomes quit unequal.

In this study, we propose an efficient method to realize the dynamic load balance for large-scale DEM simulations. By applying the slice-grid method in two directions, it is found that each domain has the same number of particles during the whole simulation time. In addition, several techniques of GPU memory management have been developed to move particles to the neighbor GPUs across the domain boundary. We demonstrate some DEM simulation as shown in from Fig.1 to Fig4, a golf bunker shot using 130 million particles with 256 GPUs, a conveyer with screw, a spiral slider and so on, carried out on TSUBAME supercomputer in Tokyo Institute of Technology.

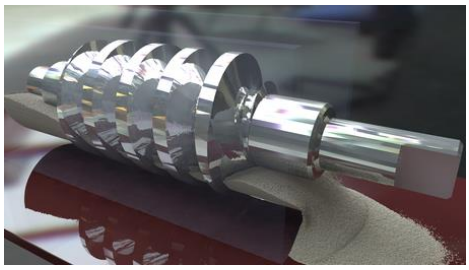


Fig1. Conveyer with screw

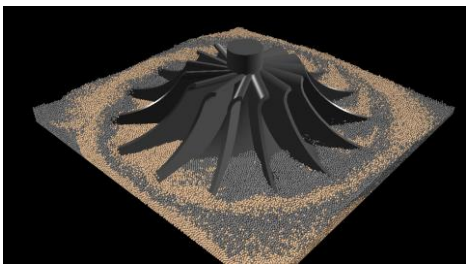


Fig2. Agitation simulation

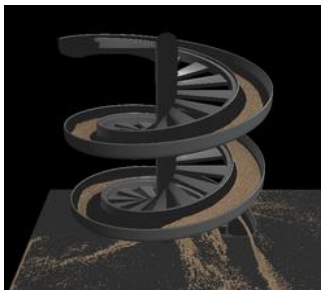


Fig3. Spiral slider

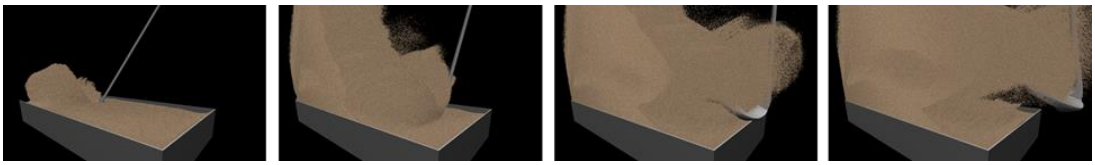


Fig4. Demonstration of 130 million particles golf-bunker shot

3P

Block BiCGStab for lattice QCD on the K computer

H. Suno[1,2], Y. Nakamura[1], K.-I. Ishikawa[3], and Y. Kuramashi[1,4,5]

[1]RIKEN Advanced Institute for Computational Science, Kobe 650-0047, Japan,

[2]RIKEN Nishina Center, Wako 351-0198, Japan,

[3]Graduate School of Science, Hiroshima University, Hiroshima 739-8526, Japan,

[4]Graduate School of Pure and Applied Science, University of Tsukuba, Ibaraki 305-8571, Japan,

[5]Center for Computational Science, University of Tsukuba, Ibaraki 305-8577, Japan,

We have developed a block version of the Bi-Conjugate Gradient Stabilized (BiCGStab) solver for treating the Wilson-Dirac equation with multiple right-hand sides in lattice QCD with clover fermions. We implement the QR decomposition, Lüscher's domain decomposition Schwarz alternating procedure (SAP) preconditioner and the symmetric successive over-relaxation (SSOR) iteration with *locally lexicographic* ordering for obtaining the domain inverse. Code development and optimization are carried out for the K computer at the RIKEN Advanced Institute for Computational Science. The computation kernels have been shown to improve in performance depending on the SAP block size, the number of compute nodes, and the number L of right-hand sides. The block BiCCStab solver, written in single precision, will be included as a preconditioning step for an outer BiCGStab solver in double precision. Test calculations will be performed with lattice size 96^4, using 2048 nodes of the K computer. The computational cost is found to reduce with increasing the number L of right-hand sides up to ~20%. The performance of a computational kernel exceeds 50% efficiency, and the single precision block BiCGStab has more than ~30% sustained efficiency.

4P

In-Situ Visualization Tool for PIC Simulation

Nobuaki Ohno[1] and Hiroaki Ohtani[2,3]

1. Graduate School of Simulation Studies, University of Hyogo, Japan
2. Department of Helical Plasma Research, National Institute for Fusion Science, Japan
3. Department of Fusion Science, The Graduate University for Advanced Studies (SOKENDAI), Japan

As the ability of supercomputers has been greatly improved, the size of simulation results with which the researchers have to cope has become very large. Usually they visualize and understand their results as a post process using interactive visualization software on their PCs. However, its size is becoming large for PCs, so interactive visualization on PCs will be unpractical. Therefore in-situ visualization attracts attention recently. We have developed an in-situ visualization tool for PIC (Particle-In-Cell) simulation[1], which usually produces data of particles, scalar and vector fields. This tool provides various visualization methods i.e. spheres for particles, isosurfaces, slices, volume rendering for scalar fields, and stream lines, arrows for vector fields (see Fig.1). It is written in Fortran 90 and provided as a Fortran's module, so that simulation researchers can use it by simply adding Fortran's statements in their simulation codes and linking it. It has already been tested on Plasma Simulator supercomputer at National Institute for Fusion Science in Japan. The first target of this tool is PASMO[2].

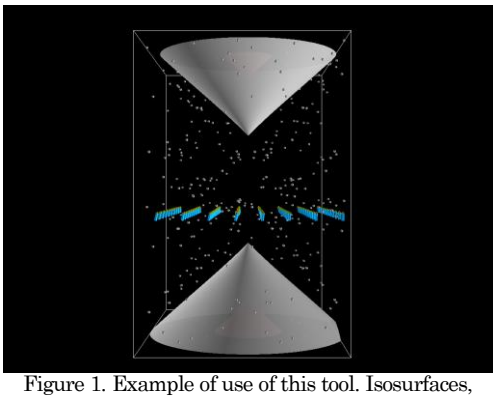


Figure 1. Example of use of this tool. Isosurfaces, arrows and spheres are used. The data is not a simulation result but was generated by using mathematical functions.

[1] C.K.Birdsall and A.B.Langdon: Plasma Physics Via Computer Simulation, McGraw-Hill, New York (1985).

[2] H.Ohtani and R. Horiuchi: Plasma Fusion Res. 4 (2009) 024.

5P

Stability Analysis of Plane Wave Propagation for Investigation of Liquefaction Triggering Condition

Jian CHEN, Hideyuki O-tani and Muneo Hori
Computational Disaster Mitigation and Reduction Research Unit,
Advance Institute for Computational Science, RIKEN

Liquefaction refers to the change of ground behavior from solid-like to fluid-like. By virtue of decades of endeavors, general consensus has been arrived on liquefaction: a phenomenon caused by the *coupling* of soil particles and ground water. Extensive experimental studies have shown that, in the process of liquefaction, the water pressure increases, with the weakening of the soil strength. Despite the progresses made in experimental and numerical studies, the triggering condition of liquefaction remains *unknown*: It is difficult to measure directly the weakening of the soil contact in experiments; the dynamics of water is oversimplified in numerical simulations. In this paper, we study theoretically and numerically the hypothesis that *loss of stability* is the triggering condition of liquefaction. Through stability analysis of the governing equations for plane wave propagation, we show that the *anisotropy* of material property, which models the dilatancy of soil, determines the stability of the solutions. Instability occurs when the anisotropy rate is large. Consistent results from numerical simulations based on particle discretization are obtained.

6P

Supporting Workflow Management of Scientific Applications by MapReduce Programming Model

Shinichiro Takizawa
Riken AICS

There are many applications that run many tasks as a workflow, such as ensemble simulation and data processing, in scientific applications. We surveyed various applications that run on large scale parallel systems, extracted their workflow patterns and then investigated requirements for building the workflow on the MapReduce programming model. To fulfill the requirements, we implemented necessary mechanism to 'K MapReduce' MapReduce implementation. To illustrate the scientific applications' workflows on the MapReduce model, we implemented two application workflows on the K MapReduce; Replica exchange molecular dynamics and Genome analysis. As a result of comparison with implementations without MapReduce, we confirmed a performance benefit in the former case and a coding benefit in the latter case.

7P

Data Assimilation with error-correlated observations

Koji Terasaki, Takemasa Miyoshi

Data assimilation Team, Research Division, AICS, RIKEN

In data assimilation in numerical weather prediction, the treatment of observation error is one of the essential issues. The observation-error covariance matrix is assumed to be diagonal in most of the data assimilation systems. However, radiosondes, for example, observes meteorological variables at different levels with the same instrument, so that it would have correlated errors in observed data. In this study, experiments are performed using a toy model to investigate the role of the observation error correlations. The results indicate the analysis error is dramatically improved by using correlated observation-error.

8P

Investigation of the novel data I/O concept considering the use of non-volatile RAM for massively large-scale numerical simulation

Shohei Onishi † Shingo Hashikawa †† Yukihisa Suzuki †
† Tokyo Metropolitan University †† Technology Joint Corporation

Recently, according to the development of computational performance due to the many core systems for example GPGPU, MIC and so on, the I/O bottleneck appeared in massively large-scale scientific simulation. To avoid that I/O bottleneck, some studies on how to introduce non-volatile RAM (NVRAM) in computer architecture have been conducted. In these studies, NVRAM is used as the substitute for main memories or storage devices.

In this paper, we propose the novel I/O concept for the computer architecture substituting NVRAM for conventional volatile memory i.e. DRAM as main memory. To investigate feasibility of the concept, we construct pseudo system consists of InfiniBand™ network and several computer nodes, and design libraries and APIs for this system. The I/O performance was measured for this preliminary constructed system.

As a result, write and read performance are approximately 1.3 GB/s and 0.7 GB/s, respectively. Our proposed I/O system was able to improve I/O performance compared to conventional file I/O from (to) solid state drive (SSD) connected by the SATA 3.0 interface. Write and read performance of our proposed system were increased by 170% (x2.7) and 70% (x1.7), respectively, than those of SSD.

9P

A Bayesian optimization approach to multi-model ensemble data assimilation

Shigenori Otsuka and Takemasa Miyoshi
RIKEN Advanced Institute for Computational Science

Multi-model ensemble data assimilation has been explored to account for uncertainties of numerical models using different dynamical cores and physics parameterizations. In the previous studies, the ensemble size for each model is prescribed subjectively, and the typical choice is the uniform distribution, in which each model has an equal ensemble size. In this study, we adopt a discrete Bayesian filter to a multi-model ensemble Kalman filter (EnKF) to find the optimal ensemble sizes for each model. As a first step, we test the proposed approach with the Lorenz 40-variable model.

Different values of the model parameter F are used to mimic the multi-model ensemble. The true F is chosen to be 8, and the observations are generated by adding independent Gaussian noise to the true time series. When the multi-model ensemble consists of F = 6, 7, 8, 9, 10, the Bayesian filter finds the true model and converges to F = 8 quickly. When F = 6, 7, 9, 10 (i.e., the multi-model ensemble does not contain the true model), the closest two models F = 7 and 9 are selected.

We developed an effective inflation method to make the Bayesian filter work without converging to a single imperfect model. Covariance inflation factors computed by an adaptive inflation method in EnKF is used as a measure to modify the ensemble size. How much we flatten the ensemble sizes is controlled by a tuning parameter (ß) of the system. The strength of temporal smoothing of the ensemble size (1/κ) is another tuning parameter.

When the multi-model ensemble contains the true model, the performance for smaller ß values is almost the same as that of the manually-tuned multi-model ensemble. When the multi-model ensemble does not contain the true model, the best combination of the tuning parameters is κ=1.1 and ß=0.6.

10P

Data Assimilation

- synergizing simulations and data -

Takemasa Miyoshi
RIKEN Advanced Institute for Computational Science, Kobe, Japan

Computational science is now commonly considered the third mode of science, complementing and adding to experimentation/observation and theory. More recently, the “Fourth Paradigm” has been known as the data-centric science, in which “Big Data” play a key role. Data assimilation connects simulations and experimentation/observation data by extracting the most from both to optimize the simulation accuracy and experimentation/observation strategy. This poster presentation will include my group’s research activities on data assimilation in numerical weather prediction, as well as my future perspective for “Big Data Assimilation” that connects extreme-scale simulations and next-generation sensors.

11P

A High-productivity Framework for Multi-GPU Computing of Weather Prediction Code

Takashi Shimokawabe
Tokyo Institute of Technology

Numerical weather prediction is one of the major applications in high-performance computing and is accelerated on GPU supercomputers. Obtaining good parallel efficiency using more than thousand GPUs often requires skillful programming, for example, both MPI for the inter-node communication and NVIDIA GPUDirect for the intra-node communication. The Japan Meteorological Agency is developing a next-generation high-resolution meso-scale weather prediction code ASUCA. We are implementing it on a multi-GPU platform by using a high-productivity framework for mesh-based application. Our framework automatically translates user-written functions that update a grid point and generates both GPU and CPU codes. The framework provides C++ classes to describe stencil access pattern, loop calculation and GPU-GPU communication easily and effectively. The framework can also hide the complicated implementation for the efficient communications described above. The programmers write user's code just in the C++ language and can develop program code optimized for GPU supercomputers without introducing complicated optimizations for GPU computation and GPU-GPU communication. In this presentation, we will show the implementation of the weather prediction code by using this framework and the performance evaluation on the TSUBAME 2.5 supercomputer at Tokyo Institute of Technology.

12P

Work Sharing with GPU and CPU on PGAS Programming Language XcalableMP-dev

Tetsuya Odajima[1], Taisuke Boku[1,2], Mitsuhisa Sato[1,2], Toshihiro Hanawa[2],
Yuetsu Kodama[1,2],Raymond Namyst[3], Samuel Thibault[3], Olivier Aumage[3]

[1] Graduate School of Systems and Information Engineering, University of Tsukuba

[2] Center for Computational Sciences, University of Tsukuba

[3] University of Bordeaux - LaBRI - INRIA Bordeaux Sud-Ouest

We have been researching a framework to enable the work sharing of parallel processing by the coordination of CPUs and GPUs on hybrid PC clusters based on the high-level parallel language XcalableMP-dev[1]. Original XcalableMP enables high-level parallel programming with directives that support data distribution and loop/task distribution among multiple nodes on a distributed memory parallel systems such as PC clusters. XcalableMP-dev is an extension of XcalableMP for a hybrid PC cluster, where each node is equipped with accelerated computing devices such as GPUs, many-core environments.

On the work sharing among GPUs and CPU cores on such clusters; it is an important issue to decide the optimal load balance among these heterogeneous computing resources. Through the development in [1], we found the necessity of adaptive load balancing for GPU/CPU work sharing to achieve the best performance for various application codes.

In this poster, we enhance our language system XcalableMPdev/StarPU to add a new feature which can control the task size to be assigned to these heterogeneous resources dynamically during application execution. As a result of performance evaluation on several benchmarks, we confirmed the proposed feature correctly works and the performance with heterogeneous work sharing provides up to about 40% higher performance than GPU-only utilization even for relatively small size of problems.

[1] T. Odajima, T. Boku, T. Hanawa, J. Lee, and M. Sato. GPU/CPU Work Sharing with Parallel Language XcalableMP-dev for Parallelized Accelerated Computing In *Sixth International Workshop on Parallel Programming Models and Systems Software for High-End Computing (P2S2)*, pages 97–106, Sept. 2012.

13P

Characteristic dynamics of a financial market

Takashi Shimada
Department of Applied Physics, Graduate School of Engineering,
The University of Tokyo

Dynamics of real complex systems has attracted broad interest. Social and economical systems are becoming good object for this issue, because of their rapidly accumulating quantitative data. The lack of stationarity and large noise are the difficulties we typically face on such data.

Here we introduce our recent approach on US stock market data to understand its characteristic dynamics. From the correlations of stock returns in about past 20 years, we define several typical *states*. Using those *states,* we find that the change of the market structure looks rather intermittent, not gradual.

(Reference)
M. C. Mnnix, T. Shimada, F. Leyvraz *et al.,* Scientific Reports **2** 644 (2012).
http://www.nature.com/srep/2012/120910/srep00644/full/srep00644.html

14P

Parameter sensitivities of the dual-localization approach in the SPEEDY-LETKF

Keiichi Kondo, Takemasa Miyoshi and Hiroshi L. Tanaka
Graduate School of Life and Environmental Sciences, University of Tsukuba
RIKEN Advanced Institute for Computational Science

In the ensemble Kalman filter, covariance localization plays an essential role in treating sampling errors in the error covariance between distant locations. Excessive localization may limit the influence of observations. Miyoshi and Kondo (2013) proposed the dual-localization approach, which analyzes the high-resolution and low-resolution components separately. The high-resolution component is computed from the full-resolution ensemble perturbations with tight localization and has a detailed structure of the error covariance. The low-resolution component captures longer-range covariance structures using the spatially-smoothed reduced-resolution perturbations and large-scale localization. The dual-localization approach has two tuning parameters: the short and long localization scales and the choice of the smoothing function. In this study, the dual-localization approach is applied to the SPEEDY-LETKF system, and we investigate the parameter sensitivities. The SPEEDY model (Molteni 2003) is a T30/L7 atmospheric general circulation model (AGCM) with intermediate complexity.

Twin experiments with the SPEEDY model are performed under the perfect model scenario. The ensemble size is fixed at 20. CTRL experiment employs the traditional LETKF with a 700-km horizontal localization parameter after manual optimization (Kang, personal communication). The other experiments employ the dual-localization approach (DLOC) with different choices of smoothing functions and localization parameters. DLOC has two types of smoothing functions. One is the spectral truncation at 21 wavenumbers with the spherical harmonics, and the other is the Lanczos filter (Lanczos 1956) with the critical frequency f_c = 1/5, 1/8 and 1/11. The localization parameters are chosen by 100 km increment from 300 km to 900 km for the short localization, and 600 km to 1300 km for the long localization.

Results suggest that the dual-localization approach outperforms the traditional single localization with relatively wide choices of the two localization scales by about 400 km ranges. Similar results were obtained with DLOC using either the spherical harmonics or the Lanczos filter if the smoothing strengths are similar. As the degree of smoothing becomes stronger, the optimal localization parameters shift to larger scales, and the shaded area becomes smaller.

15P

Performance Evaluation on Nuclear Simulation Code GT5D on HA-PACS

Norihisa Fujita †, Hideo Nuga ‡, Taisuke Boku †, ‡, Yasuhiro Idomura*
† Graduate School of Information Engineering, University of Tsukuba
‡ Center for Computational Science, University of Tsukuba
* Japan Atomic Energy Agency

Within recent important computation engineering fields, the nuclear fusion simulation for experimental reactors is one of the important applications. Moreover, due to very high resolution of space decomposition for accurate simulation, the number of grids in a target system has been growing extremely large for recent target reactor size. In this research, we will port one of the largest and latest nuclear simulation codes named GT5D to GPU clusters.

It aims to analyze the turbulence phenomena in tokamak plasma. GT5D is written in Fortran and parallelized in a hybrid combination of OpenMP and MPI. We use PGI CUDA Fortran to port it. We optimize it for GPU clusters with multiple GPUs on a node. Based on the profile result of GT5D on a CPU node, we decide to offload the whole of the time development part of the program to GPUs except MPI communication. bcdf is a function to exchange data of halo around decomposed domain. Splitting the calculation around bcdf function into the boundary area and the inner area, we optimized its communication to make overlapping with calculation. We archived 3.37 times faster performance in maximum in function level evaluation, and 2.03 times faster performance in total than the case of CPU-only execution, both in measurement on high density GPU cluster HA-PACS where each computation node consists of four NVIDIA M2090 GPUs and two Intel Xeon E5-2670 (SandyBridge) to provide 16 cores in total. These performance improvements on single GPU correspond to four CPU cores, not compared with a single CPU core. It includes 53% performance gain with overlapping the communication between MPI processes with GPU calculation.

16P

HA-PACS/TCA

Yuetsu Kodama, Taisuke Boku, Toshihiro Hanawa, Mitsuhisa Sato
Center for Computational Sciences, University of Tsukuba

HA-PACS (Highly Accelerated Parallel Advanced system for Computational Sciences) is the latest generation of HPC system not only as the commodity GPU cluster, but also as the demonstration system for research and development of an efficient accelerating computing. In the HA-PACS project, target applications, including particle physics, astrophysics, and life sciences applications, are predetermined. We have been servicing HA-PACS base cluster from Feb. 2012. It is a commodity GPU cluster whose node consists of two Intel Xeon E5-2670 CPUs and four NVIDIA M2090 GPUs, and total 268 nodes are connected by dual IB QDRx4 network with full bisection bandwidth. In the project, we also developed an experimental system as a proprietary interconnection network connecting accelerators over the nodes. In usual GPU clusters, inter-node communication among accelerators requires several memory copies via CPU memory, and the communication latency causes severe performance degradation. In order to address this problem, we propose the Tightly Coupled Accelerators (TCA) architecture to reduce the communication latency between accelerators over different nodes by directly exchanging PCIe packets between nodes. We developed PEACH2 board for realizing the TCA architecture using FPGA. We adopted Altera's Stratix IV GX FPGA, which includes four PCIe Gen2 x8 ports as the hard IP. The PEACH2 chip provides fast operation for the relay function of the PCIe packets and sophisticated DMA functions, such as the chaining mechanism by hard-wired logic. In Oct. 2013, the HA-PACS/TCA cluster, which includes 64 compute nodes (each of which has two Xeon E5-2680v2, four K20X GPUs, an InfiniBand host adaptor, and a PEACH2 board), was installed. Sub-clusters which consist of 16 nodes are connected by PEACH2 network. We will demonstrate the effectiveness of the TCA architecture on this system.

17P

Template-Based Automatic Construction of Building Models from GIS data

Hideyuki O-tani, Jian Chen, Muneo Hori
RIKEN Advanced Institute for Computational Science

Integrated Earthquake Simulation (IES) is a seamless simulation of the three phases of earthquake in an urban area, namely, strong ground motion generation, seismic structure response, and human/community disaster actions. In IES, building models in an urban area and an earthquake scenario are used as input, and the resultant disaster is computed objectively. In order to make building models necessary to IES, We have developed a new methodology to make seismic response analysis models from GIS data. It is based on a template-based shape recognition method applied to floor shapes extracted from GIS data. In this methodology, an adequate number of prescribed templates are precomposed, and one of them is selected to adapt each floor shape which is composed of a set of polygons. Since the differences between templates and floor shapes can be easily calculated using grid data with boolean values, the template-based approach enhances the robustness of floor shape recognition and automatic construction of building models.

18P

Evaluation of parallel GPU application using Tightly Coupled Accelerators

Hisafumi Fujii[1] , Toshihiro Hanawa[2] , Yuetsu Kodama[1,2] ,
Taisuke Boku[1,2] , Mitsuhisa Sato[1,2]

[1] Graduate School of Systems and Information Engineering, University of Tsukuba

[2] Center for Computational Sciences, University of Tsukuba

In recent years, heterogeneous clusters using accelerators are widely used for high performance computing system. In such clusters, the inter-node communication among accelerators requires several memory copies via CPU memory, and the communication latency causes severe performance degradation. To address this problem, we propose Tightly Coupled Accelerators (TCA) architecture to reduce the communication latency between accelerators over different nodes. In addition, we promote the HA-PACS project in Center for Computational Sciences, University of Tsukuba not only in order to build up HA-PACS base cluster system, as the commodity GPU cluster, but also in order to develop the experimental system based on TCA architecture, as the proprietary interconnection network connecting among accelerators beyond the nodes.

We preliminary evaluated the performance of TCA using parallel GPU benchmark. We selected the Himeno benchmark that perform the calculation of fluid stencil code. In Himeno benchmark, it is required to exchange data in boundary region between GPU over the nodes. TCA enables direct communication between GPU memory over the nodes using hardware RDMA. Also, once DMA descriptor is written, TCA can start communication by just kick DMAC every time because the regions to be communicated are statically defined in this benchmark. Therefore, the cost of communication is low. In the case that the problem size is small, the execution with TCA communication was 1.44 times faster than the execution using MVAPICH2 that supports CUDA.

19P

Conformational change of SERCA upon alternating protonation states in Ca^{2+}-binding site

Chigusa Kobayashi[1] and Yuji Sugita[1,2,3]
[1]RIKEN, AICS, [2]RIKEN QBiC, [3]RIKEN, TMS

Sarcoplasmic reticulum Ca^{2+}-ATPase (SERCA) is a representative P-type ATPase. The protein pumps Ca^{2+} from muscle cell to lumen by alternating Ca^{2+} affinity of Ca^{2+}-binding site. Proton counter-transport plays a quite important role in the transport against a large concentration gradient. Experimental studies revealed the conformational change as changing Ca^{2+} affinity at the higher pH. They also postulated that change of protonation states in the binding site brings the conformational change. To understand how SERCA utilize proton counter-transport for Ca^{2+} transport, we performed molecular dynamics simulations of SERCA with different protonation states by using all-atom model. We show that proton transfer from the binding site induces the conformational change of important acidic residues and opens of water channels as pathway of Ca^{2+}.

20P

Deep moist atmospheric convection in a sub-kilometer global simulation: Critical resolution towards the resolving the deep convection

Yoshiaki Miyamoto*, Yoshiyuki Kajikawa, Ryuji Yoshida, Tsuyoshi Yamaura,

Hisashi Yashiro, and Hirofumi Tomita

RIKEN Advanced Institute for Computational Science

Modeling the global atmosphere is a great challenging issue. One of most significant difficulties in the global models arises in representation of clouds, especially deep moist convection[1]. The convection is a key element of the weather and climate system for transporting mass, momentum, and thermal energy. However, it has been impractical to simulate convection realistically in global models, because of the large gap in scales between convection[2,3] (10^0 km) and global motions (10^4 km). We successfully conducted the first ever sub-kilometer global simulation and successfully described the features of convection. Our grid-refinement simulations revealed that the necessary resolution for simulating convection is less than about 2.0 km. The convection structure, number of convective cells, and distance to the nearest convective cell dramatically changed at this resolution. The reason for this is that the convection core was resolved using multiple grids in simulations with resolutions less than 2.0 km.

21P

Metadynamics: Implementation in GENESIS and Demonstration of Efficient Simulations

Raimondas Galvelis[1] and Yuji Sugita[1,2,3]

[1] RIKEN Advanced Institute for Computational Science

[2] RIKEN Theoretical Molecular Science Laboratory

[3] RIKEN Quantitative Biology Center

Metadynamics (MTD) is an accelerated sampling algorithm aiming to maximize the output of molecular dynamics (MD) simulations. MTD, by design, is capable of the efficient simulation of biosystems with large energetic barriers and rough energy landscape within the limited time scale of MD simulations, and it is applicable to arbitrary large systems and complex phenomena (i.e. folding, binding, chemical reactions, etc.). Our implementation of MTD in GENESIS is focused toward scalability to utilize massively-parallel computers (i.e. "K computer"). The accuracy and efficiency is demonstrated with several simulations of biomolecules and compared with an another established accelerated sampling method, replica-exchange umbrella-sampling (REUS).

22P

"Identity Parareal" for Time-evolution Problems

Toshiya TAKAMI and Daiki FUKUDOME
Research Institute for Information Technology, Kyushu University, Japan

While the spatial domain decomposition is considered as one of the convincing techniques for large-scale computing problems, the number of decompositions is limited for modest scales since the communication cost becomes relatively large. Then, another direction for the domain decomposition, e.g., the time axis, should be considered to achieve strong scaling on massively parallel computers. One of the prominent methods to realize the time-domain decomposition is the "parareal-in-time" algorithm [1]. Since it is a general algorithm to ensure time-domain parallelism, it can be applied to various large-scale scientific time-evolution problems [2].

However, there are several shortcomings in the original parareal-in-time algorithm. In order to overcome them, we introduce a new implementation called "Identity Parareal" (iParareal) to achieve effective time-parallel computations, where an identity transformation is used as a coarse solver [3, 4]. In our poster, we present convergence properties (See Fig. 1) and speedups of the iPararel method applied to scientific problems. We will also discuss efficient configurations of scientific computations in exa-scale computing.

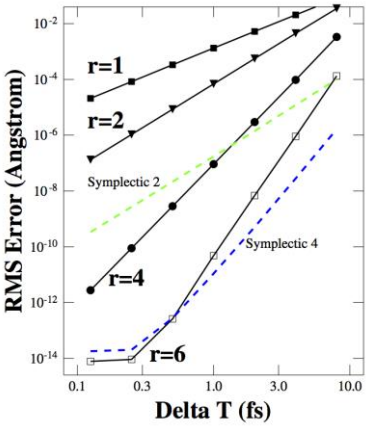


Fig. 1: Convergence property of the iPararel method.

[This work is supported by JST, CREST.]

Reference

[1] J.-L. Lions, Y. Maday, and G. Turinici, *A 'parareal' in time discretization of PDE's*, C. R. Acad. Sci. Ser. I Math., vol.332, 661-668 (2001).
[2] R. Speck, D. Ruprecht, R. Krause, M. Emmett, M. Minion, M. Winkel, and P. Gibbon, *A massively space-time parallel N-Body Solver*, SC12, Tech. Paper No. 92, 1-11 (2012).
[3] T. Takami and D. Fukudome, *An Efficient Pipelined Implementation of Space-Time Parallel Applications*, ParCo'13, Sep. 10-13, Munich (2013).
[4] T. Takami and D. Fukudome, *A Simple Implementation of Parareal-in-Time on a Parallel Bucket-Brigade Interface*, PPAM'13, Sep. 8-11, Warsaw (2013).

23P

Molecular orbital calculation for efficient SIMD operations by means of multiple geometry inputs

Hiroaki Honda[a,d], Yuichi Inadomi[b,d], and Jun Maki[c]

[a] *Research Institute for Information Technology, Kyushu University, 6-10-1 Hakozaki, Higashi-ku, Fukuoka 812-8581 Japan*

[a] *Graduate School of Information Science and Electrical Engineering, Kyushu University, 744 Motooka Nishi-ku, Fukuoka 819-0395 Japan*

[c] *Institute of Systems, Information Technologies and Nanotechnologies, 2-1-22, Momochihama, Sawara-ku, Fukuoka, 814-0001, Japan*

[d] *JST-CREST*

Introduction

In order to build up exascale computer systems, it is imperative to use many-core processors, which will have 16 or larger-ways SIMD functional units from requirements of high performance and low power consumption. However, conventional Hartree-Fock programs have quite low SIMD operation level parallelism for the two-electron Fock-matrix (G-matrix) calculation which is the bottleneck of RHF program, since there are many complex data-dependencies for primitive molecular integral calculations in the G-matrix code. In this research, we propose a Hartree-Fock method which calculates multiple-inputs of different molecular geometries in parallel, and those calculations are applied for SIMD parallel operations. We evaluate maximum performance for our method with test inputs whose molecular geometries are same.

Parallel Hartree-Fock calculation for multiple molecular geometry inputs

Generally, for improving SIMD operation efficiency, target program has to be implemented as follows: (1) array elements of multiple-input data are aligned as continuous memory addresses for efficient vector-load and store operations, (2) data are aligned in adequate memory address boundaries, and (3) array notations are utilized for the SIMD operation regions. According to these rules, we implemented the G-matrix calculation of multiple molecular geometry inputs.

Performance evaluations

We evaluated our proposed methods by three types of desktop computers with 2-way SIMD Xeon X5650, 2 and 4-way SIMD E5-2650, and 8-way SIMD Phi processors. For parallel G-matrix computations, we achieved 1.82, 1.97 and 5.84 times speed-ups for Intel Xeon X5650, E5-2650, and Phi processor computers, respectively. According to the results of hardware counter data, 99.7% and 94.0% of double precision floating points are computed by Xeon X5650 and E5-2650, respectively. It is expected that multiple-input parallel calculation will improve the SIMD operation efficiency for practical calculations of potential energy surfaces.

24P

The Simulation Study of the Interaction between Transmembrane Region of Amyloid Precursor Protein and Cholesterols

[1,2]Naoyuki Miyashita, [3]Fumiko Ogushi, [1,2,4]Yuji Sugita
[1]RIKEN QBiC, [2]RIKEN AICS, [3]Ochanomizu University, [4]RIKEN

Bio-membrane consists of several types of lipids and membrane proteins. Such mixed membrane sometimes forms micro-domains, which are called Raft. The Raft contains Cholesterols and Sphingomyelins mostly. It affected the ability of the association between membrane proteins and so on. Amyloid Precursor Protein (APP) is also affected by the Raft. This protein plays a very important role in the early stage of Alzheimer's disease. Amyloid beta peptide, which is related to the senile plaque, is produced from APP by beta- and gamma-secretase. Recently, the structure of the transmembrane domain of APP (APP TM) has been determined by the NMR spectroscopy [1,2]. The experiments have also indicated the cholesterol binding residues. However, it is not clear how cholesterols bind to the APP in the Raft. We report the relation between cholesterols and a small membrane protein, APP and WALP23, in the raft like environments, using Martini Coarse Grained (CG) model simulations [3,4]. The simulation results have supported the experimental observations of the cholesterol binding sites in the APP TM. Our results suggested that two or three cholesterols bind to the APP simultaneously. The cholesterols are favorable to APP rather than WALP23. We propose that the APP affects the cholesterols too. It provides the heterogeneous membrane bilayer environments as the different number of cholesterols in the upper or the lower layer of the membrane.

[1] P. J. Ballet et al., SCIENCE, 2012, 336, 1168-1171
[2] K. D. Nadezhdin et. al., Acta NATURE,2011, 3, 69-76
[3] S. J. Marrink et al., J. Phys. Chem. B, 2007, 111, 7812-7824
[4] S. O. Yesylevskyy et al., PLoS Comput Biol, 2010, 6, e1000810

25P

Krylov subspace methods for computing correlated Brownian noise vectors in Brownian dynamics simulations with hydrodynamic interactions

Tadashi Ando

Laboratory for Biomolecular Function Simulation
Computational Biology Research Core
RIKEN Quantitative Biology Center (QBiC)

Brownian dynamics is a molecular simulation algorithm that can incorporate hydrodynamic interactions between particles. In the simulations, a Cholesky factorization is commonly used to compute correlated Brownian noise vectors. However, this factorization is an $O(N^3)$ operation for an N-particle system, which is generally the bottleneck in the Brownian dynamics. Here, we study methods based on Krylov subspace approximations for computing Brownian noise vectors to overcome this difficulty. We show that the computational time of Krylov subspace methods scales very nearly as $O(N^2)$ without any loss of simulation accuracy. Thus, Krylov subspace methods are recommended for performing large-scale Brownian dynamics simulations with hydrodynamic interactions.

26P

Midpoint cell method for hybrid (MPI+OPENMP) parallelization of molecular dynamics

Jaewoon Jung[1], Takaharu Mori[2,3], and Yuji Sugita[1,2,3]

[1]*Computationl Biophysics Research Team, RIKEN AICS, Kobe 640-0047, Japan*
[2]*Theoretical Molecular Science Laboratory, RIKEN, Wako 351-0198, Japan*
[3]*Quantitative Biology Center, RIKEN, Kobe 640-0047, Japan*

e-mail: jung@riken.jp

We have developed a new method for hybrid parallelization (MPI+OPENMP) in molecular dynamics (MD) simulation using midpoint cell with cell-pair Verlet list. As usual domain decomposition MD program, the global simulation space is divided to sub-domains for different MPI processors. Each sub-domain is again divided into cells, which are utilized as interaction cell pairs for nonbonded calculations.

The midpoint cell approach keeps the advantages of the original midpoint method : (1) It applies not only to pairwise interaction but also to interactions involving more than two particles, (2) It communicates equal amount of data in each direction, leading more effective communication links in certain network topologies like 3D torus, and (3) We could avoid communication to support charge spreading and force interpolation in PME using sufficient large cutoff values. Keeping the advantage of the midpoint method, our midpoint cell scheme has additional merits : (1) Suitable for shared memory parallelization, leading efficient hybrid parallelization, (2) Improvement of the locality by storing particle data cell-wise, and (3) Filtering out unnecessary calculations of midpoint checking procedure.

The parallel performance of the midpoint cell scheme is tested on K computer, showing scalability up to 32,768 and 262,000 cores for systems of 1 million atoms and 100 million atoms, respectively. One MD time step with long-range interaction could be carried out within 4 milliseconds even for 1 million atoms systems with particle mesh Ewald (PME) electrostatics.

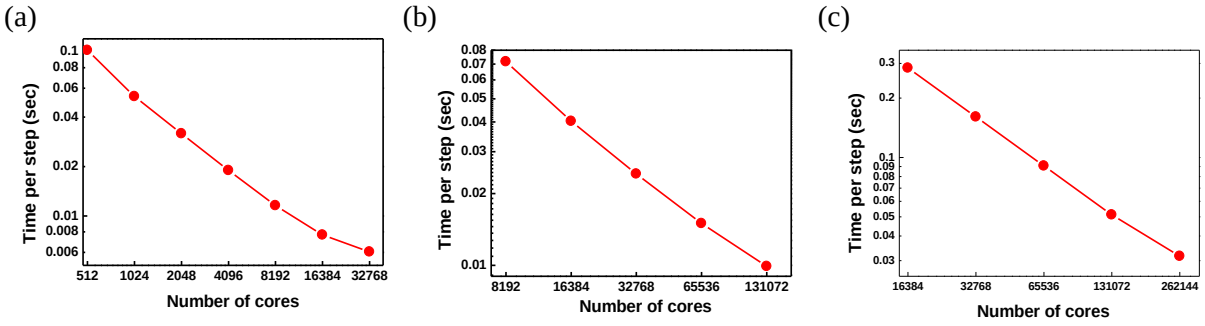


Figure. Parallel performance of systems of (a) 1.3 M, (b) 11.2M, and (c) 100M atoms.

27P

GPU accelerated Fock matrix preparation routine in OpenFMO

Hiroaki Umeda, Toshihiro Hanawa, Mitsuo Shoji, and Taisuke Boku
Center for Computational Sciences, University of Tsukuba

GPU accelerated Fock matrix preparation routine for the fragment molecular orbital (FMO) calculation has been implemented into the OpenFMO program. We proposed atomic-addition-less Fock matrix preparation algorithm to share Fock matrix among threads in a thread block, and implemented it on GPGPU with CUDA. With several speedup techniques, our program showed 3.3 times faster performance with a GPU card and 4 CPU cores than the case without GPU on the HA-PACS GPU cluster, where it is equipped with two Intel E5 CPUs (Sandy Bridge-EP, 2.6GHz) and four NVIDIA M2090 GPUs on a node. And furthermore, this performance is better than the GPU accelerated program, LIBCCHEM, in the GAMESS program.

We also perform benchmark calculation with K20 GPU card. The performances are remarkably improved from that with M2090 GPU, especially for the two-electron integral types with higher angular momentum.

Acknowledgements:
This study is partially supported by Ministry of Education, Culture, Sports, Science and Technology (MEXT), and also supported by the project "Research and Development on Unified Environment of Accelerated Computing and Interconnection for Post-Petascale Era" of Basic Research Programs: CREST "Development of System Software Technologies for post-Peta Scale High Performance Computing," Japan Science and Technology Agency.

28P

An XML-based Programming Framework for User-defined Code Transformations

Hiroyuki Takizawa[1,2], Xiong Xiao[1,2], Shoichi Hirasawa[1,2],
and Hiroaki Kobayashi[1]
1 Tohoku University, 2 JST CREST

In this project, we develop an XML-based programming framework, named Xevolver. The framework exposes an abstract syntax tree (AST) in an XML data format to programmers. Hence, the programmers can adopt various XML-related technologies to transform, analyze, and visualize application codes. The current implementation of the framework employs XSLT to define application-specific code transformations. To annotate application codes for the custom code transformations, the framework allows programmers to define OpenMP-like compiler directives in another XML file. Accordingly, an AST, custom compiler directives, and their code transformation rules are all represented as XML documents. By incrementally inserting the custom compiler directives, a real application can be migrated to another system without significantly modifying the original code, because custom code translation rules are written in an external XSLT file. We can change the behaviors of the directives for individual systems by changing XSLT rules in the external file. Accordingly, we can evolutionarily improve the application so as to have high performance portability without messing up the original code.

29P

Materials design on the lithium-ion and sodium-ion conductors by molecular orbital calculation

Taku Onishi
Department Chemistry for Materials, Graduate School of Engineering,
Mie University
E-mail: taku@chem.mie-u.ac.jp

Abstract

Lithium-ion conductors have attracted much interest, due to developments of materials for a next-generation secondary battery. Previously, we clarified the mechanism of lithium-ion conduction in perovskite-type compounds, by the use of molecular orbital calculation, combined with density functional theory (DFT). In addition, we designed one of the best lithium ion conductors. In this presentation, we also introduce the recent research on sodium ion conductor.

References

[1]T. Onishi, Adv. Quant. Chem. 64, 31-81 (2012)
[2]T. Onishi, Solid State Ionics 180, 592-597 (2009)
[3]T. Onishi, Polyhedron 28, 1792-1795 (2009)
[4]T. Onishi, Int. J. Quant. Chem. 109, 3659-3665 (2009)
[5]T. Onishi, Int. J. Quant. Chem. 112, 3777-3781 (2012)

30P

Possibility of a single biomolecule structure determination by X-ray Free Electron Laser

Atsushi TOKUHISA
RIKEN/AICS

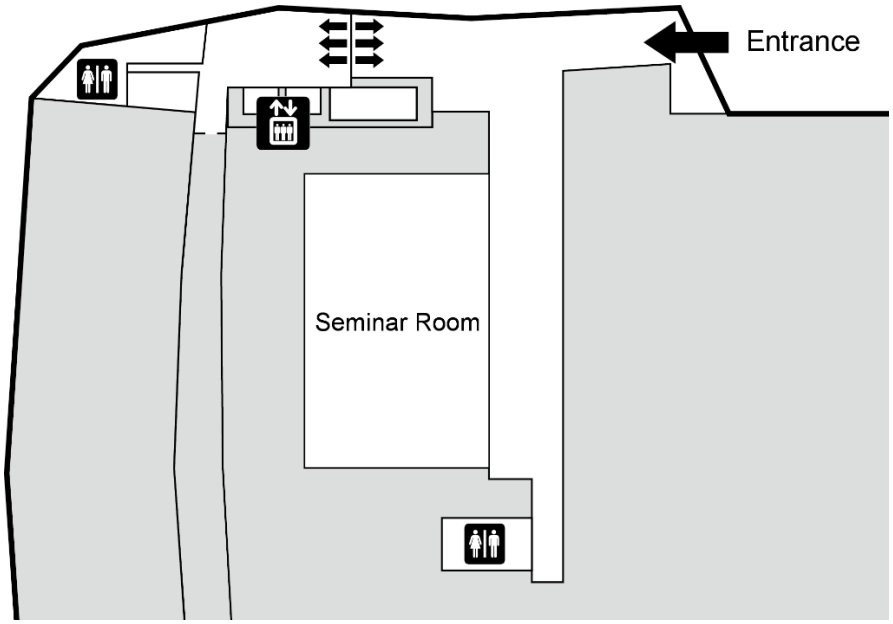
X-ray free electron laser generates intense X-ray laser with very short pulse. This new light source offers new possibilities of biomolecule imaging. One of the promising is single-particle coherent diffraction imaging (CDI).

In single-particle CDI, high intensity femto-second X-ray laser is irradiated onto a target of a single biomolecule with random orientation, and two-dimensional coherent diffraction patterns are recorded repeatedly, each time for a different orientation. One of the most difficulty points is that the diffraction intensity is very weak even if using XFEL. We proposed an algorithm for classifying and assembling two-dimensional noisy diffraction patterns to improve S/N ratio of diffraction patterns and construct 3D diffraction pattern. The algorithm enables to extract signals necessary to construct an atomic-resolution three-dimensional structure from data deeply immersed in the quantum noise. By analyzing about one million diffraction patterns, we can achieve sub nano meter structural resolution using our algorithm.

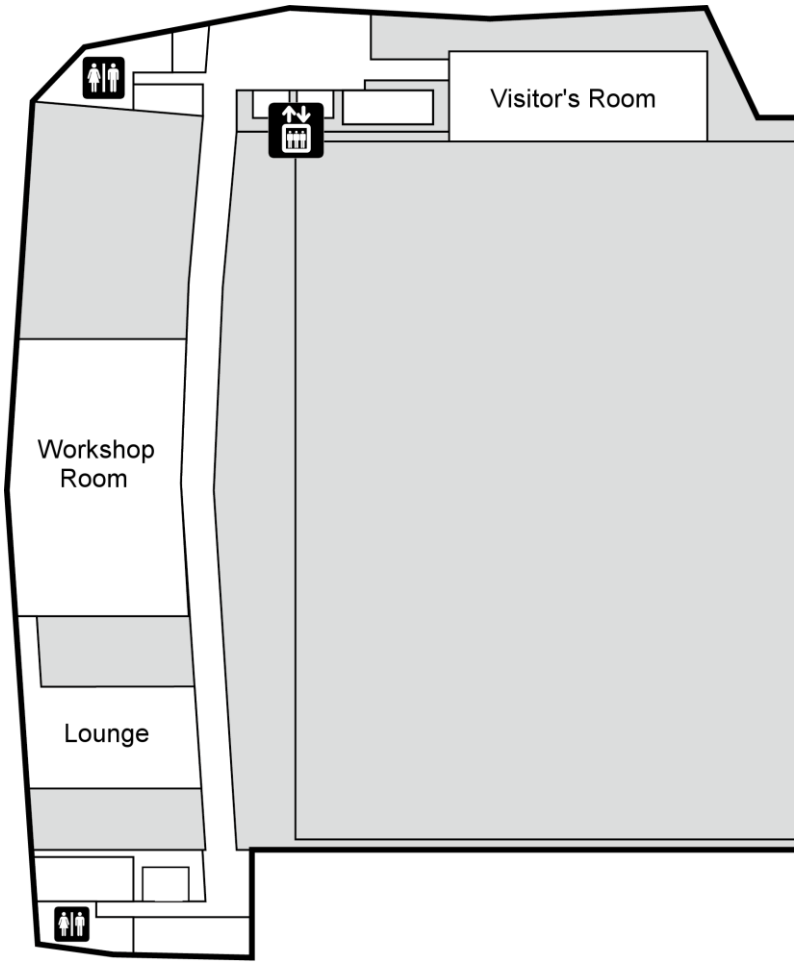
On the other hand, in the current experimental status, we can obtain only low resolution data set because of the absence of efficient sample delivery system. Therefore, we are developing a methodology for structure determination using currently available data set. To compensate low resolution data set, we assume structure models from simulation and perform diffraction pattern matting by using a similarity detection algorithm (Tokuhisa et al., 2012, Acta Cryst A. 68. 336-381). We report current status of our effort.

Floor Map

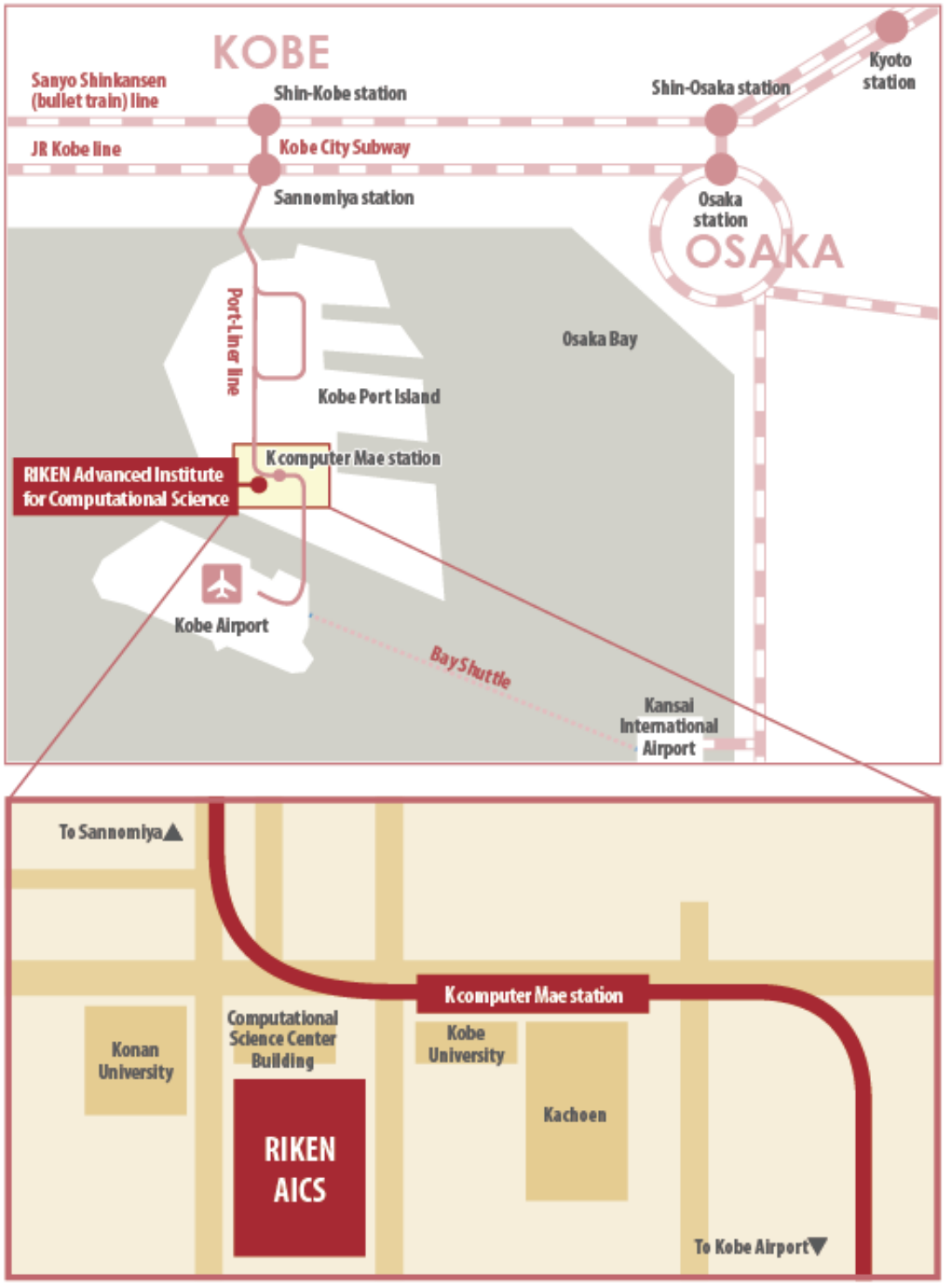
1st floor



6th floor



Area Map


KOBE
Sanyo Shinkansen (bullet train) line
Shin-Kobe station
Shin-Osaka station
Kyoto station
JR Kobe line
Kobe City Subway
Sannomiya station
Osaka station
OSAKA
Port-Liner line
Osaka Bay
Kobe Port Island
K computer Mae station
RIKEN Advanced Institute for Computational Science
Kobe Airport
Bay Shuttle
Kansai International Airport
To Sannomiya
K computer Mae station
Konan University
Computational Science Center Building
Kobe University
Kachoen
RIKEN AICS
To Kobe Airport

The Fourth
AICS International Symposium

Computer and Computational Sciences for Exascale Computing

Editor & Publisher

RIKEN Advanced Institute for Computational Science (RIKEN AICS)

7-1-26, Minatojima-minami-machi, Chuo-ku, Kobe, 650-0047 JAPAN

E-mail: aics-sympo-staff@riken.jp

http://www.aics.riken.jp/

Published December, 2013