AICS

RIKEN Advanced Institute for Computational Science

ANNUAL REPORT

FY2013-14

AICS Research Activities
July 2014

RIKEN

K computer

Computer simulations
create the future

Contents

Preface

More than four years have passed since the RIKEN AICS was established. It is my pleasure to report our research and development activities of AICS during the period of April 2013 to March 2014. This report focuses on the activities of Research Division as well as those of Operations and Computer Technologies Division.

As of March 2014, the numbers of research teams and units of the Research Division have amounted to 16 and 3, respectively. The total number of researchers in the division has grown to more than 100 to date. The research division has been designed to cover both various computational sciences and some aspects of computer science, and collaborations and co-design of computational sciences and computer science have been very much encouraged at its inception.

The main mission of the Operations and Computer Technologies Division is to operate and manage the K computer to serve it to HPC users smoothly and efficiently. Among the four teams in the division, this report focuses on System Operations and Development Team (SODT) and Software Development Team (SDT). Analyzing the operational statistics collected during the use of the K computer, SODT improves the system functions such as job scheduling, file systems, and users' environments. The main activities of SDT are three-fold: analysis and optimization of real applications, user supports, and performance evaluation of middleware systems used or to be used for the K computer.

July 2014

Akinori Yonezawa
Director, Research Division
RIKEN Advanced Institute for Computational Science (AICS)

Mission and Overview

Japan's Third Science and Technology Basic Plan (a Cabinet resolution adopted in March 2006) designated next-generation supercomputing as a key technology of national importance that should be the focus of investments in gestation periods for large-scale national projects. As a result, RIKEN along with the Ministry of Education, Culture, Sports, Science and Technology (MEXT) are putting full efforts into the development and advancement of such technology.
Under the guidance of MEXT and on the basis of the "Law on Joint Use Promotion of Large-Scale Advanced Research Facilities" (effective July 2006), RIKEN has been managing the construction of the Next-Generation Supercomputer, the "K computer." The K computer is to be a shared resource based on the above law and, with its wide accessibility, is expected to be put to a broad range of uses—from diverse fields of basic science and technology research to applications in industry. It was with this in mind that RIKEN established the Advanced Institute for Computational Science (AICS) on July 1, 2010. Through the use of its world-class supercomputer boasting 10 petaflops of computational power, and through collaboration and integration of the fields of computational science and computer science, AICS strives to create an international center of excellence dedicated to generating world-leading results. AICS's missions are:

1. Operating the K computer efficiently for users of wide research areas as well as of industries,
2. Carrying out the leading edge research of computational science and technology, and establishing itself as the COE of computational sciences in Japan.
3. Proposing the future directions of HPC in Japan.

And also, AICS's missions include:

- Promoting strong collaborations (or co-development) between computational and computer scientists, working with the core-organizations of the strategic areas identified by the Strategic Programs for Innovative Research (SPIRE),
- Raising and promoting young scientists who are strong in both computational and computer sciences, and
- Pursuing new concepts for the future HPC beyond the petascale (including exascale).

The research teams of AICS are carrying out the leading edge research of computational science and technology, and also expected to provide useful software to the users of the K computer.

Today's supercomputers including the K computer employ hundreds of thousands of cores which work simultaneously and in parallel to rapidly calculate and process enormous volumes of data. Getting a supercomputer to work at its full potential, however, requires extremely sophisticated technology.

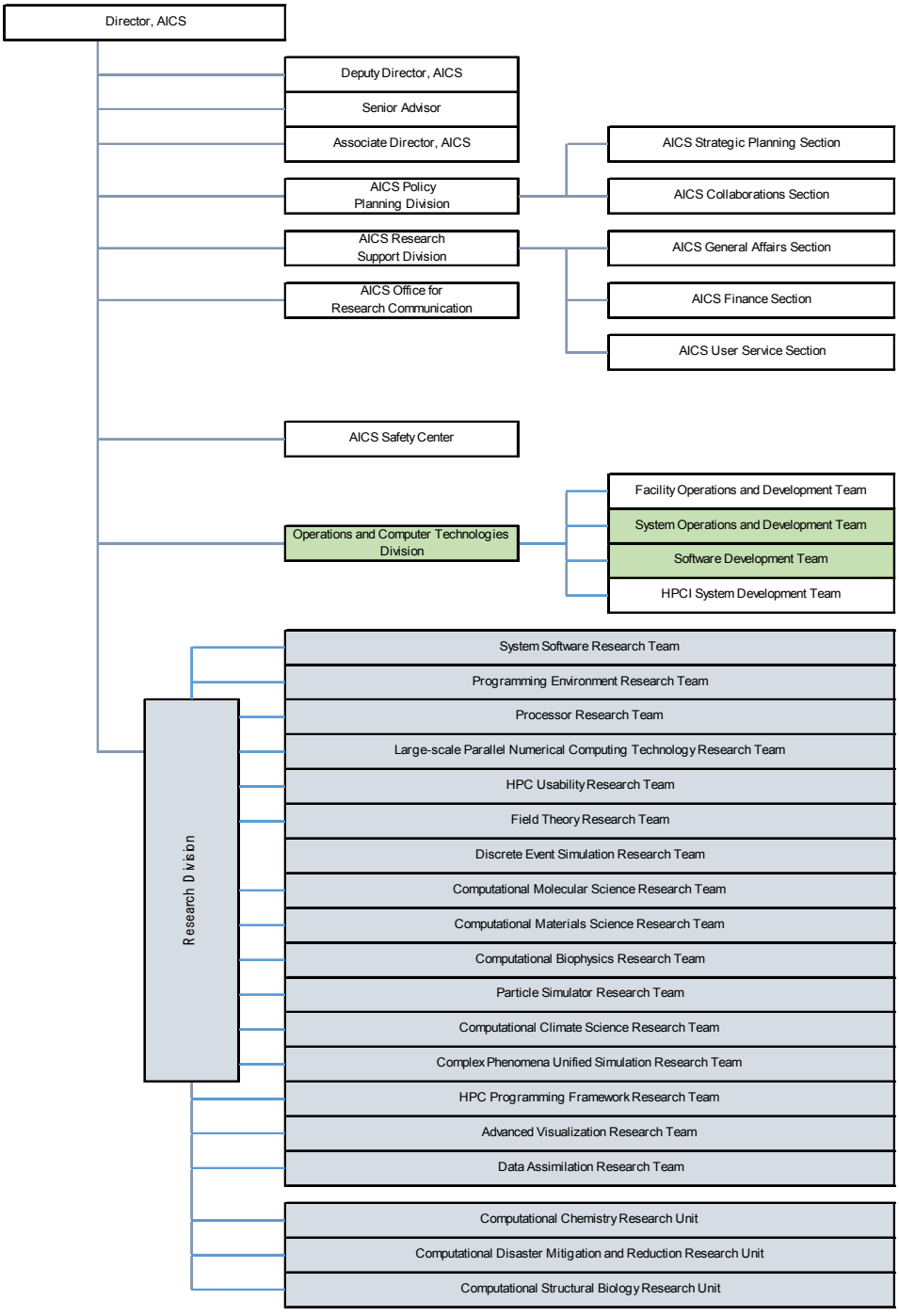
Achieving this kind of technology is impossible without close collaboration between computational and computer science. Computational science involves the application of new methodologies of large-scale numerical simulation for research and development in physics, chemistry, biology, medical science, and engineering. Computer science, on the other hand, focuses on computer systems architecture, the algorithms that lay out the methods and procedures for problem-solving, management of computational and memory resources, systems software that allows communication among different computers, and application programs.

The AICS Research Division brings together researchers specializing in computational and computer science to merge and develop the two fields into what may eventually become a whole new field of interdisciplinary computational science that will maximize the potential of the supercomputer for major breakthroughs in science and technology.

The Operations and Computer Technologies Division of AICS is engaged in research and development of advanced operation technologies of the K computer as well as its surrounding facilities and advanced system software of the K computer to make more effective use of its computing resources.

Organization

The organization of AICS (as of March 2014) is schematically shown below. The research teams in computer science and computational sciences are closely integrated into the Research Division. Operations of the K computer and researches on its advanced utilization technologies are conducted in the Operations and Computer Technologies Division.



System Software Research Team

1. Team members

Yutaka Ishikawa (Team Leader)
Atsushi Hori (Senior Scientist)
Keiji Yamamoto (Postdoctoral Researcher)
Akio Shimada (Research Associate)
Yoshiyuki Ohno (Research Associate)
Masayuki Hatanaka (Research Associate)
Toyohisa Kameyama (Technical Staff)

2. Research Activities

The system software team focuses on the research and development of an advanced system software stack not only for the "K" computer but also for towards exascale computing. There are several issues in carrying out future computing. Two research categories are taken into account: i) scalable high performance libraries/middleware, such as file I/O and low-latency communication, and ii) a scalable cache-aware, power-aware, and fault-aware operating system for next-generation supercomputers based on many core architectures.

Parallel file I/O is one of the scalability issues in modern supercomputers. One of the reasons is due to heavy metadata accesses. If all processes create and write different files, the metadata server receives so many requests by all processes not only at the creation time but also at writing data to each file. Three approaches have been conducted to mitigate this issue. One approach is to introduce a file composition technique that gathers multiple data generated by an application and stores these data into one or a few files in order to reduce the number of files accessed by processes. Another approach is to provide multiple metadata server in which the requests for metadata are sent to a metadata server resolved using hash function. The third approach is to provide a smart MPI-IO implementation for applications using MPI-IO functions.
Increasing number of cores and nodes enforces strong scaling on parallel applications. Because the ratio of communication time against local computation time increases, a facility of low-latency and true overlapping communication and computation communication is desired. A communication library, integrated to the MPI library implementation in K computer, has been designed and implemented, that utilizes DMA engines of K computer. Each compute node of K computer has four DMA engines to transfer data to other nodes. If a communication library knows communication patterns in advanced, it may utilize the DMA engines. Indeed, the feature of MPI persistent communication allows the runtime library to optimize data transfers involved

in the persistent communication using the DMA engines.

System software stack developed by our team is designed not only for special dedicated supercomputers, but also for commodity-based cluster systems used in research laboratories. The system will be expected to be used as a research vehicle for developing an exascale supercomputer system.

3. Research Results and Achievements

3.1. PRDMA (Persistent Remote Direct Memory Access)

The goal of this research is to design and evaluate an efficient MPI implementation for neighborhood communication by taking advantage of the Tofu interconnect, which has multiple RDMA (Remote Direct Memory Access) engines and network links per MPI process. The neighbor communication pattern is commonly used in the ghost (or halo) cell exchanges. For example, the SCALE-LES3 includes the multiple stencil computations for weather and climate models. So, the neighborhood communication is a dominant communication pattern within the SCALE-LES3. Specifically, it is the two dimensional 8-neighbors ghost cell exchanges with periodic boundary conditions. Also, it occupies about ten percent of the execution time. Nowadays, supercomputers using three-or-higher dimensional torus have been deployed, such as the Blue Gene / Q and the K computer. For instance, the Torus Fusion (called Tofu) interconnect employed by the K computer has 6 dimensional torus and mesh as a physical topology and its node controller has 4 RDMA engines and 10 network links. These networks are possible to improve the neighborhood communication performance when MPI ranks are properly mapped on the network topology and the transfer requests are properly scheduled on the multiple RDMA engines. Unfortunately, the transfer-scheduling algorithm in the default MPI implementation provided on the K computer uses a simple round-robin method to distribute the transfer requests among the multiple RDMA engines. For neighborhood communication on the Tofu interconnect, there are major two scheduling issues; (1) load imbalance and (2) network resource contentions. In the former case, the loads between RDMA engines may be imbalance if the transfer requests are distributed to RDMA engines in round-robin fashion. In the latter case, the network link is congested if a network link is shared by some outgoing messages at the same time. Also, Contention of the RDMA engine in the receiver side occurs if some incoming messages try to request the same RDMA engine of the receiver side at the same time. Especially, the sender must specify the receiver-side RDMA engine explicitly in the RDMA transfer request of the Tofu interconnect. However, it is not clear how to distribute the receiver-side RDMA engines among senders.

Proposed Scheduling Algorithm

One of the straightforward ways to solve these scheduling issues is to model as a two-dimensional strip-packing problem. For simplicity and speed, we selected the Bottom-Left heuristic algorithm to solve this packing problem. The Bottom-Left algorithm sorts the input RDMA commands (transfer requests), and packs them at the open bottom-most and left-most position in the scheduling table, such as (a), (b), and (c) in Figure 1. In addition, we added a constraint to avoid the network resource contentions into the basic Bottom-Left algorithm. This constraint assures that two or more RDMA commands using a same network link are not scheduled at the same time. So, in the Figure 1 (d), a rectangle indicates an RDMA command, and the rectangles with the same color indicates that these commands use the same network link. The command #4 is scheduled on the RDMA engine #2 because the contention happens if it is scheduled on the RDMA engine #3.

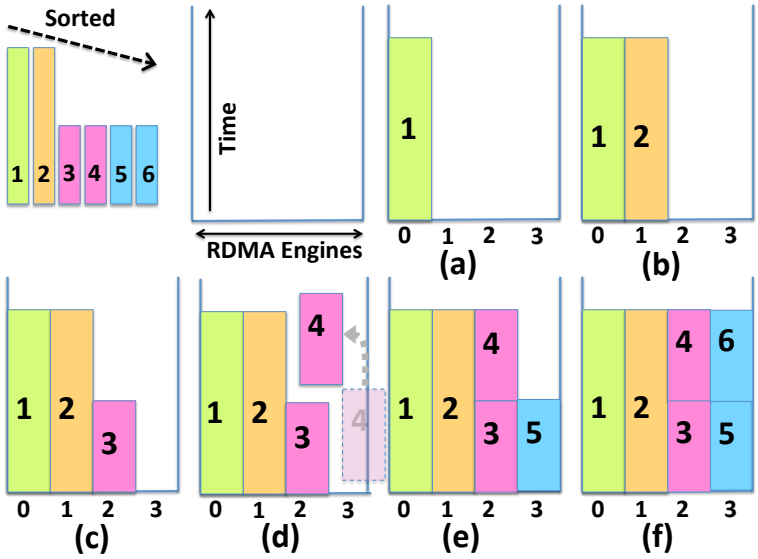


Figure 1. Scheduling by proposed Modified Bottom-Left algorithm.

Implementation and Evaluation

The proposed scheduler has been implemented and integrated into the persistent communication primitives in Open MPI on the K computer. This implementation is called PRDMA (Persistent Remote Direct Memory Access).

We measured three implementations in ghost cell exchange of SCALE-LES3: Original PC, Round-Robin, and Modified Bottom-Left. The first two implementations were measured to compare to proposed Modified Bottom-Left implementation. The first one, called Original PC, is the default Open MPI based implementation provided on the K computer. And the second one,

called Round-Robin, is the same as Modified Bottom-Left except the scheduler uses a simple Round-Robin algorithm similar to Original PC. In Figure 2, the horizontal axis shows the aggregate transfer size in a ghost cell exchange corresponding to the grid size in SCALE-LES3. The vertical left axis shows the elapsed communication time for the forty one thousands exchanges, and vertical right axis shows the percentage change against the first two implementations. The Round-Robin is 20 to 70 % better than Original PC in communication time. The Modified Bottom-Left is up to 32 % better than Round-Robin and about 50 % better than Original PC.

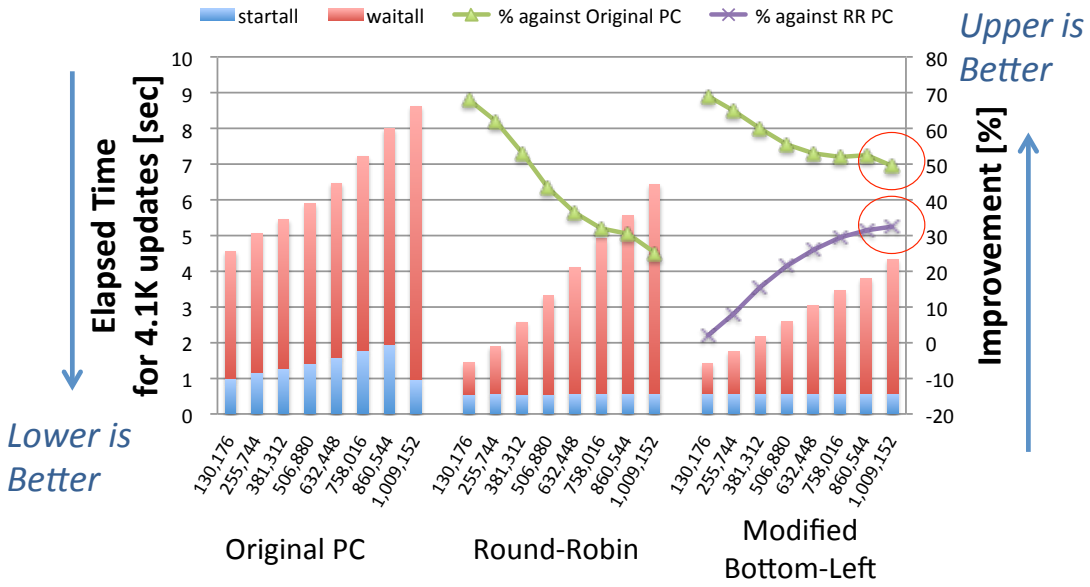


Figure 2. Evaluation of Three Scheduler implementations in Ghost Exchange.

3.2. New Process / Thread Model

Partitioned Virtual Address Space

From FY2012, we have been developing a new process / thread model that is suitable for the many-core architectures. The many-core architectures are gathering attention towards next generation supercomputing. Many-core architectures have a large number of low performance cores, and then the number of parallel processes within a single node becomes larger on many-core environments. Therefore the performance of inter-process communication between the parallel processes within the same node can be an important issue for parallel applications.

Partitioned Virtual Address Space (PVAS) is a new process model to achieve high-performance inter-process communication on the many-core environments. On PVAS, multiple processes run in the same virtual address space as described in Figure 3 to eliminate the communication overhead due to the process boundaries that the current modern OSes introduce for inter-process protection. In PVAS, the data owned by the other process can be accessed by the

normal load and store machine instructions, just like the same way accessing the data owned by itself. Then, high-performance inter-process communication is achieved.

We implemented the prototype of the PVAS process model in the Linux kernel in FY2012. We improved its quality and published it as open source software in FY 2013.

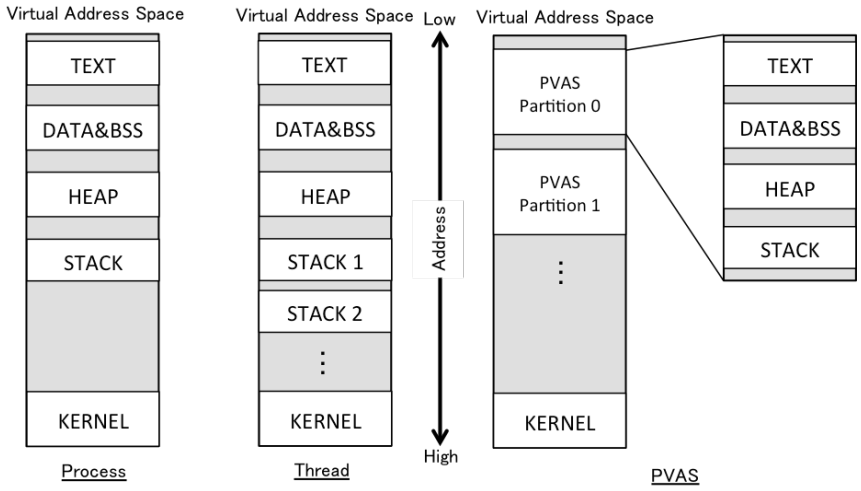


Figure 3. Semantics view of the conventional process model and PVAS.

User-level Process

Process oversubscription, which invokes a larger number of parallel processes within a computing node than the number of available CPU cores, results in better load-balance and latency hiding, and then it may improve the performance of multi-process programs. In this case, parallel processes within a computing node must be scheduled by the OS kernel. However, lightweight OS kernels that are developed for exascale systems may no longer support task scheduling, because it is one of the most resource consuming and noisy operation. In this situation, only one parallel process per CPU core is allowed, and then process oversubscription is impossible. To solve this problem, we developed user-level process. User-level process is a "process" that can be scheduled in user-space, then multiple user-level processes per CPU core can be allowed without help of OS task scheduler as described in Figure 4. Multi-process programs running on the lightweight OS kernels for exascale systems will be able to do process oversubscription by binding one parallel process to one user- level process even if those OS kernel does not support task scheduling.

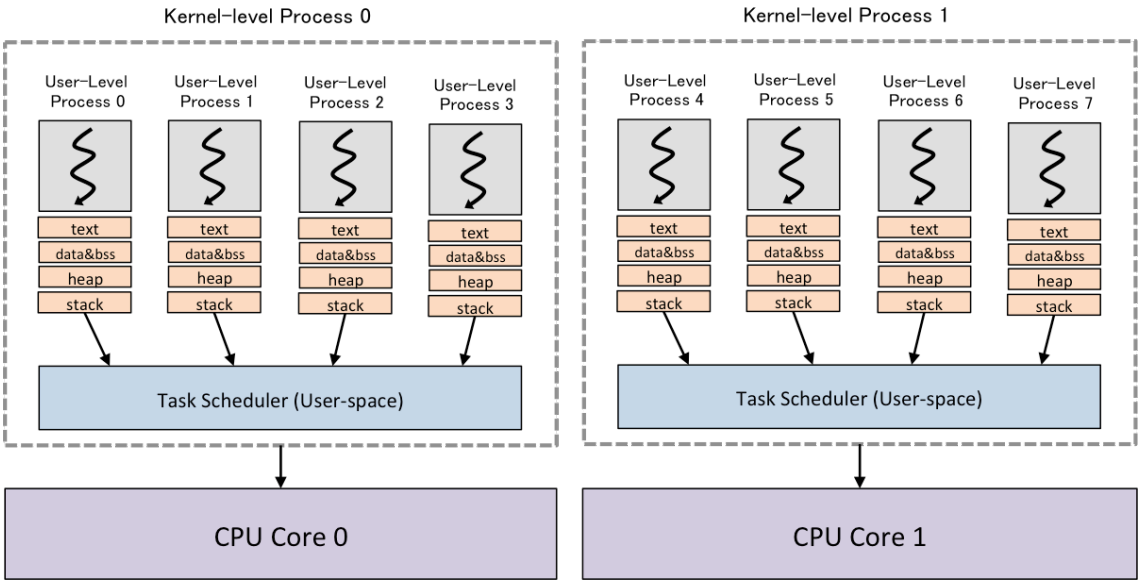


Figure 4. Semantic view of the User-level Process.

The use of user-level process also provides favorable side effects to the process oversubscription. When doing process oversubscription, the performance of context switch between parallel processes affects the overall performance of the program, because so much number of parallel processes may be invoked within a computing node. The context switch between user-level processes is faster than the context switch between traditional processes, because it is operated in user-space. As shown in Figure 5, the preliminary evaluation results show that the context switch between user-level processes is approximately 2.6 times faster than the context switch between traditional processes in the best case.

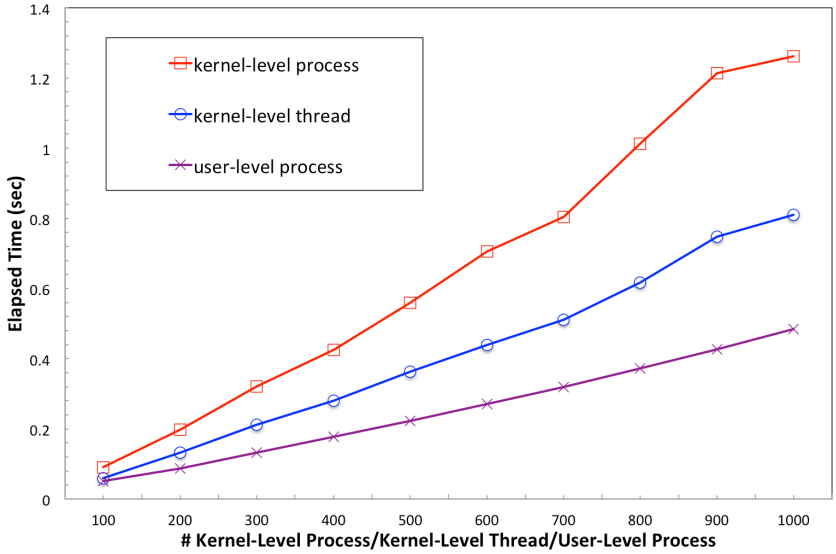
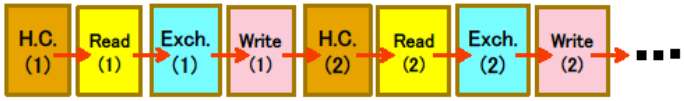


Figure 5. Elapsed time for operating 1000 times context switches.

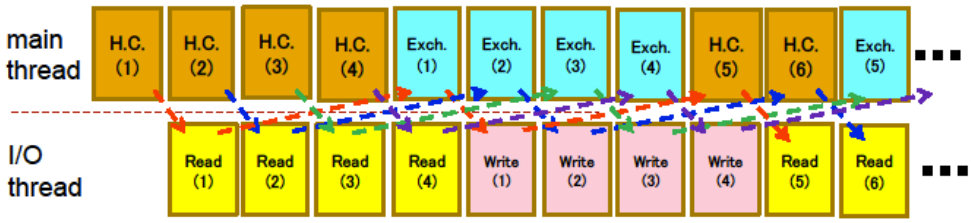
3.3. Scalable MPI-IO Using Multithreaded Scheme

A commonly used MPI-IO library named ROMIO has the two-phase I/O (TP-IO) scheme to improve collective I/O for non-contiguous accesses. This research is addressing to have a multithreaded scheme in the TP-IO in order to achieve higher performance than the original one in collective I/O for non-contiguous accesses.

In the FY2013, ROMIO in the MPICH2 library was arranged to have multithreaded operations using Pthreads. Figure 6 shows multithreaded the TP-IO operation scheme in parallel with its original scheme.



(a) Original TP-IO scheme



(b) Multithreaded TP-IO scheme

Figure 6. Original and multithreaded TP-IO in collective write operations.

Here "H.C." and "Exch." stand for hole check and data exchange phases, respectively, while "Read" and "Write" denote file read and write operations, respectively. Since every phase is processed independently in terms of access regions (described such as (1), (2) under each phase name), we can overlap read and write phases with hole check and data exchange phases as shown in Figure 6(b) using multithreaded way.

Figure 7 shows a functional diagram of the multithreaded implementation. Every MPI process invokes an I/O thread which plays file I/O using the pthread_create function. In processing I/O requests from user's MPI programs, I/O requests generated on every main thread are enqueued in the read queue in the hole check phase, followed by read operations on an I/O thread by dequeueing I/O requests from the read queue, and so on. Finally in the write phase, I/O requests are enqueued into the hole queue, then it will initiates the next hole check phase and so on. These operations are repeated until all the target regions are accessed. With the help of the

multithreaded way, ideally we can achieve at most twice the original TP-IO throughput. For further performance improvements, the multithreaded scheme introduced multiple request slots in queues. The number of slots can be managed by a key-value pair in an MPI_Info object using the MPI_Info_set function as well as the size of collective buffer size.

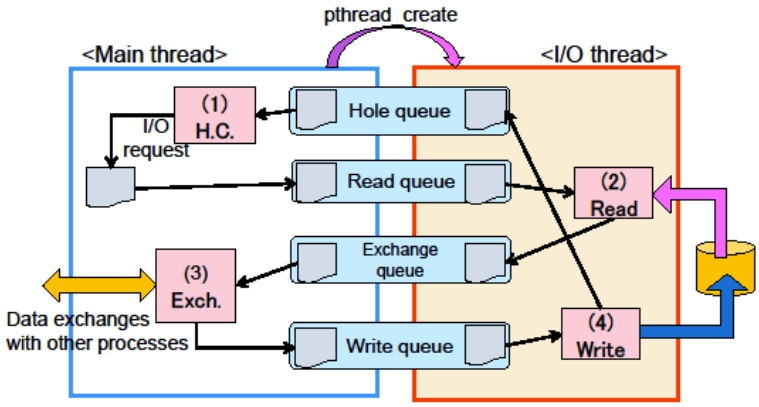
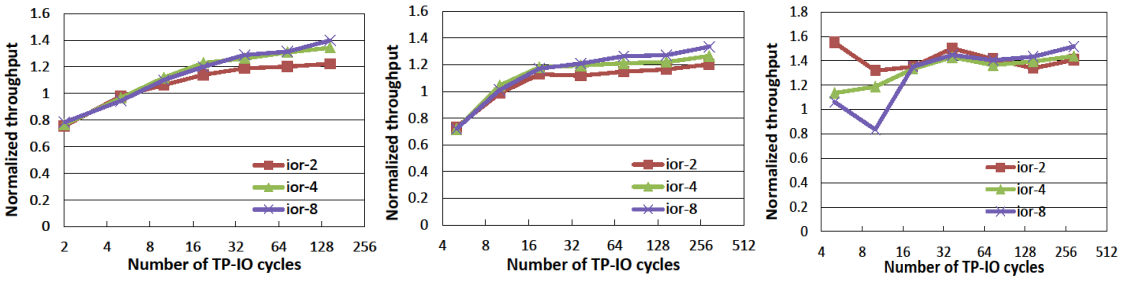


Figure 7. Functional diagram of multithreaded TP-IO.

Performance evaluation was carried out on a PC cluster system at the University of Tokyo, which is named as T2K. We used 64 PC nodes, which have 4 AMD Opteron 2.3GHz processors with 32 GiB memory using Linux kernel 2.6.18. Interconnections between PC nodes are Myrinet10G for MPI communications and the Lustre file system and Gigabit Ethernet for control. I/O operations were carried out on its Lustre filesystem version 1.8.9, which has 30 OSTs in total. In this evaluation, all the OSTs were utilized. We used HPIO benchmark, which supports unique derived data type generations required for non-contiguous I/O. ROMIO in MPICH2 version 1.4.1p1 with our multithreaded extension was evaluated. Figure 8 shows normalized write throughput relative to the original TP-IO with 64, 128, and 256 MPI processes.



(a) 64 MPI processes (b) 128 MPI processes (c) 256 MPI processes

Figure 8. Normalized write throughput of multithreaded TP-IO relative to the original one.

In every case, data block was configured with 256B data blank in each 488B data region, and absolutely 1 GiB data by multiple data blocks were generated at every MPI process. File system

cache was disabled by remounting Lustre file system prior to every MPI-IO operation run. We also changed the number of slots in queues as 2, 4, and 8, which are indicated as ior-2, ior-4, and ior-8, respectively in this figure. Horizontal axis of this figure stands for the number of TP-IO cycles, thus lower value means the larger collective buffer, while the larger value corresponds to smaller collective buffer size. Through this evaluation the multithreaded TP-IO achieved up to 60% improvements relative to the original one. Higher number of slots in queues led to higher performance gain, however it utilized larger memory resources. However, we can minimize utilized memory resources using this multithreaded scheme because this evaluation shows higher gains when we had around from 64 to 128 TP-IO cycles. It is also noticed that smaller number of TP-IO cycles led to smaller performance gain or performance degradation. This was due to imperfect overlap due to larger collective buffer size. Thus the multithreaded scheme was not effective in such case. However, such case needs larger memory resources, so the multithreaded scheme can have higher throughput gains without increasing memory utilization for collective buffer.

3.4. Big data processing on the K computer

This research is conducted by collaboration between the Data Acquisition team of RIKEN Spring-8 Center and the System Software Research team of RIKEN AICS. The goal of this project is to establish the path to discover the 3D structure of a molecule from a number of XFEL (X-ray Free Electron Laser) snapshots. The K computer is used to analyze the huge data transmitted from RIKEN Harima where SACLA XFEL facility is located. Figure 9 and Figure 10 show an outline indicating how a molecule 3D structure can be reproduced from images obtained by XFEL. Each image size is around 20 Mbytes, but may vary depending on the resolution of image sensor. The number of images required to develop a 3D structure of a molecule can be millions, resulting 20 PBytes of data size in total. Further, each image is classified into thousands of images to have every possible snapshot orientations and to reduce the quantum noise.

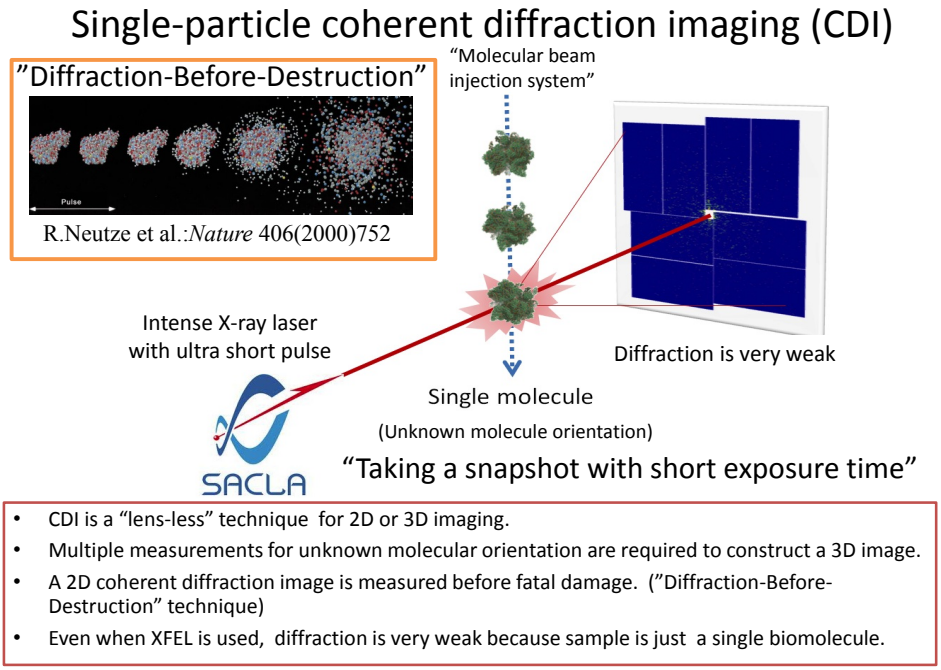


Figure 9. How SACLA XFEL works.

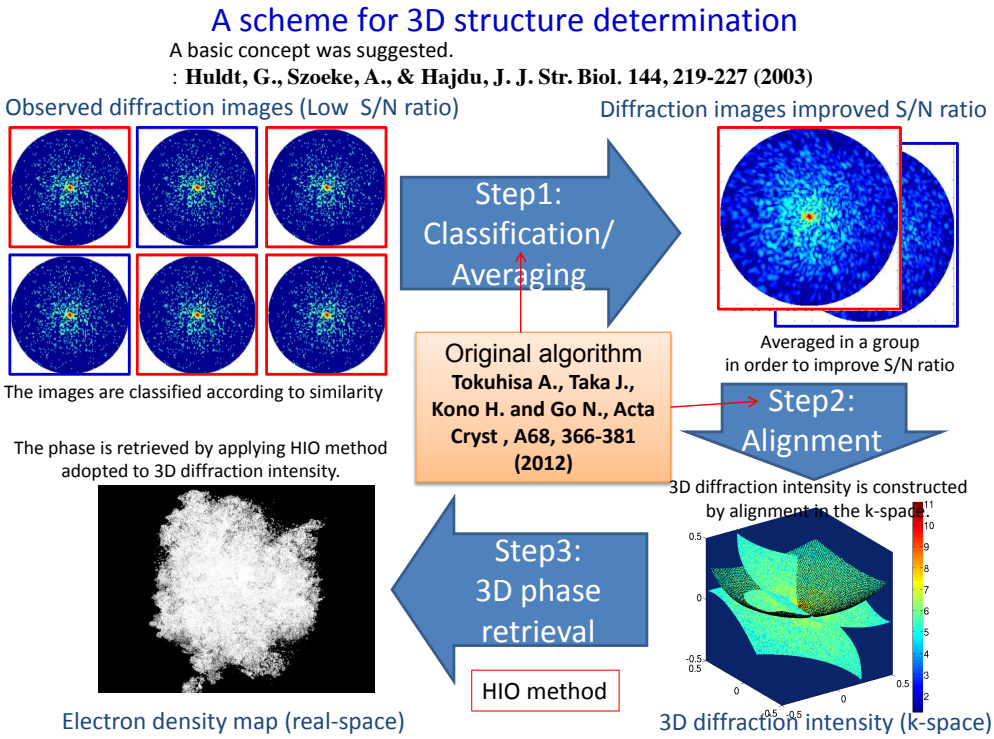


Figure 10. Obtaining electron density map from XFEL snapshots.

The developed software consists of two parts. One is to select representative images and another is to classify images using selected representative images as shown in. The classification

is conducted by several FFT operations on each image to have correlation. The order of the number of this FFT operation to select thousands classification images is $O(M^2)$, followed by the classification of the rest of the images of $O(N*M)$ FFT operations, where M is the number of classification and N is the number of images. SACLA XFEL is going to produce 30 images in a second and the time to take one million images takes approximately 9 hours. There can be the cases where the snapshots are not well enough quality to analyze. In this case, the experiment must be stopped and tuned to obtain good quality images. Thus the image analysis must be done as soon as possible. This heavy computation, one million images should be analyzed as soon as possible, requires the power of the K computer. The Data Acquisition team at SCALA has been developing a classification algorithm, while the System Software Research team at AICS has been in charge of parallelization, performance tuning, and I/O.

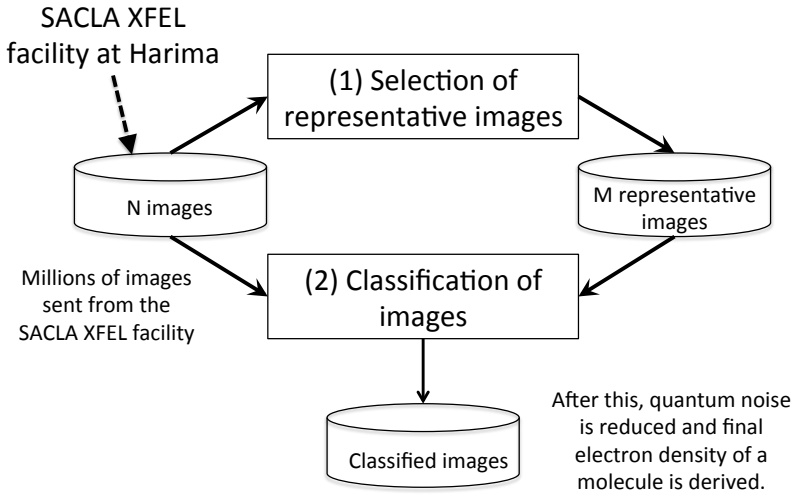


Figure 11. Block diagram of the procedure running on the K computer.

In FY2013, we optimized classification software developed in FY2012. In order to realize effective parallelization, our software keeps load balance between processes and reduces file input time by minimizing total size of the input from storage.

Figure 12 shows the workflow for classification of images. The software reads the image file only once and read images are passed to neighbors in background at every calculation step. The orange squares in Figure 12 are images which read from storage, and the greens are passed from neighbor process. The calculation is finished at N_p step, where N_p is number of processes. In addition, the software can utilize rank directory of K computer to reduce read time and increase the scalability (as shown in Figure 13). By using the software, classification for one million images can be finished in an hour on K computer.

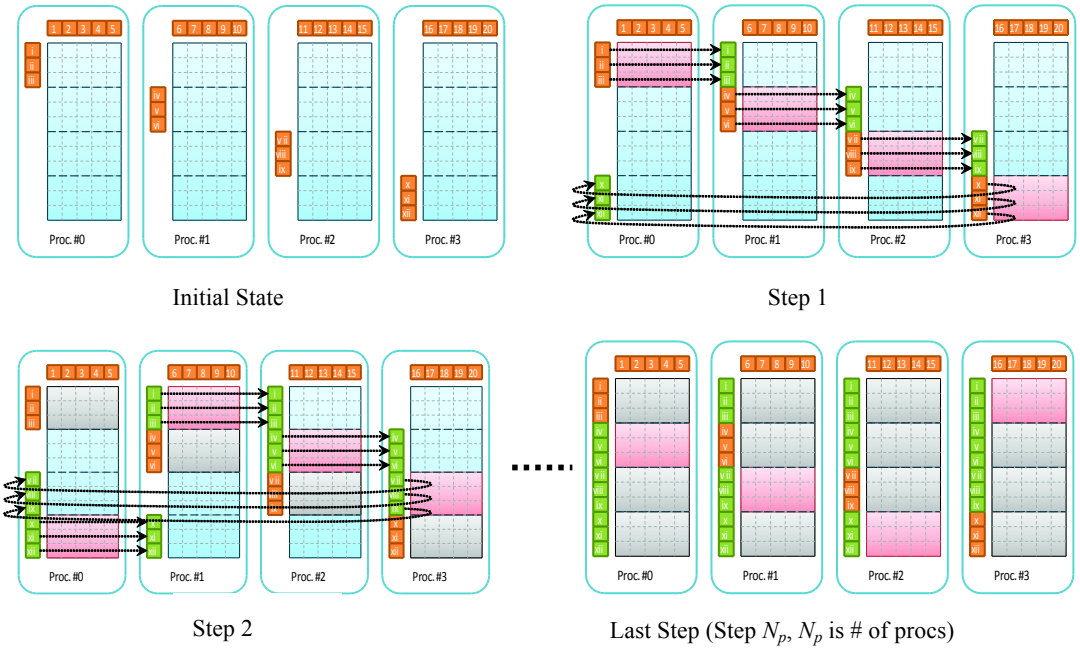


Figure 12. Calculation workflow for classification of images.

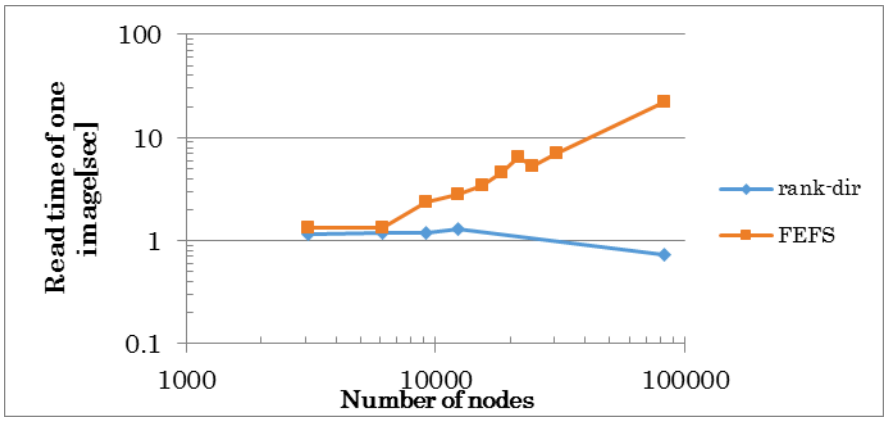


Figure 13. Read time of one image on the K computer.

3.5. File Composition Library

I/O system resources such as Meta-Data Server (MDS), Object Storage Server (OSS) and Object STorage (OST) are shared across the processes of a single parallel job. As HPC systems become large, the amount of I/O requests to each I/O system resource becomes larger, and load of them becomes heavier. The heavy loads on I/O system resources cause I/O performance degradation, and application performance degradation. It is one of the scalability issues of leadership-class high performance computing systems. We targeted the case that each process of the parallel job creates its own file and writes the file. Many parallel applications adopt this I/O pattern. Figure 14 shows the I/O performance of the K computer over the number of client processes, varying the striping counts and striping sizes (for example, "C1_S16m" indicates the striping

count is set to one and striping size is set to 16MiB). As in this figure, the bandwidth tends to decrease when the number of client processes increases. Thus, the idea of proposed "File Coordination Library" is to limit the number of client processes accessing a parallel file server simultaneously.

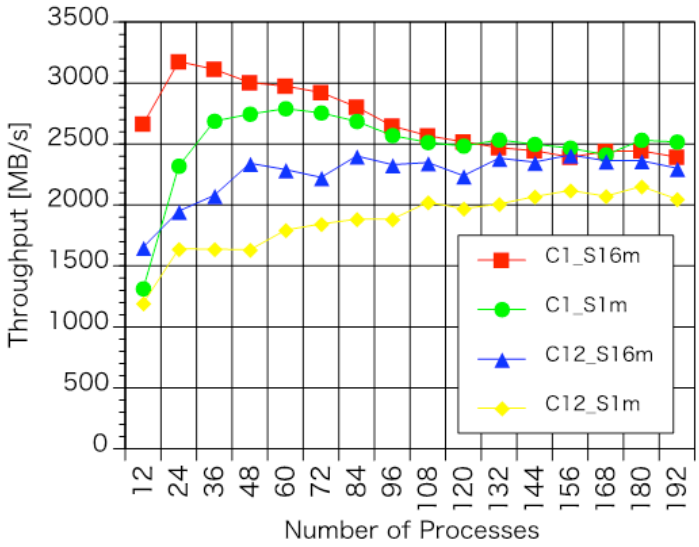


Figure 14. Write Performance over the number of client threads.

Figure 15 shows the I/O performance of the K computer with the proposed file coordination library (right graph) and without it (left graph). As shown in this figure, the average performance with the file coordination technique exhibits about 20% better.

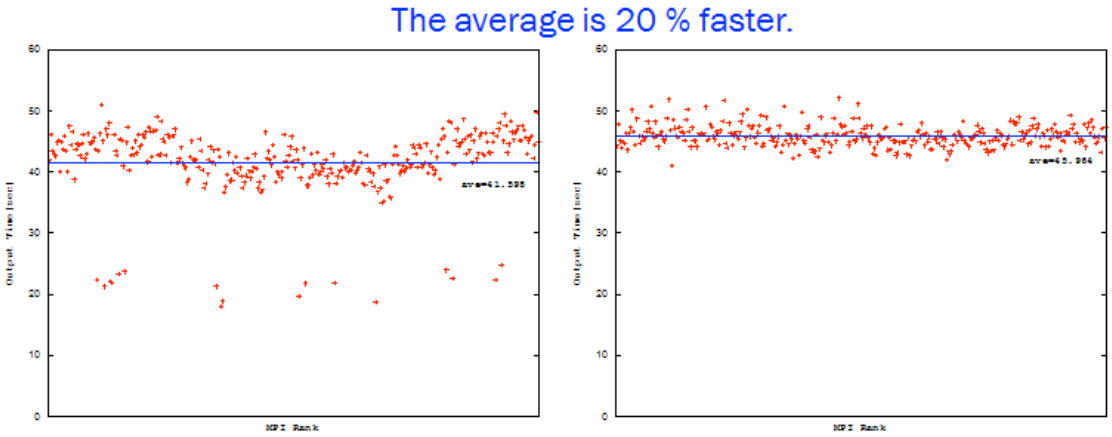


Figure 15. Write throughput of FClib.

4. Schedule and Future Plan

- Communication Library

  PRDMA (Persistent Remote Direct Memory Access) will be enhanced with a sophisticated data transfer scheduling algorithm, and it will be evaluated. MPICH3, an MPI

implementation for the MPI-3 standard, will be continued to be ported to the K computer.

- File I/O

  The classification software, developed in FY2013, processes huge image files generated by SACLA XFEL. It will be open to the users of SACLA. Based on the experience on the design of the classification software, general file I/O functions for other classification applications will be designed. The scalable MPI-IO will be adapted to the FEFS file system used in the K computer.

- New process/thread Model

  A new process/thread model, PVAS and its user-level thread, has been designed and implemented in FY2013. In FY2014, an MPI runtime environment on PVAS will be implemented and evaluated.

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] High-speed classification of coherent X-ray diffraction patterns on the K computer for high-resolution single biomolecule imaging (Atsushi Tokuhisa, Junya Arai, Yasumasa Joti, Yoshiyuki Ohno, Toyohisa Kameyama, Keiji Yamamoto, Masayuki Hatanaka, Balazs Gerofi, Akio Shimada, Motoyoshi Kurokawa, Fumiyoshi Shoji, Kensuke Okada, Takashi Sugimoto, Mitsuhiro Yamaga, Ryotaro Tanaka, Mitsuo Yokokawa, Atsushi Hori, Yutaka Ishikawa, Takaki Hatsui, Nobuhiro Go), In Journal of Synchrotron Radiation, volume 20, 2013.

[2] A Hybrid Operating System for a Computing Node with Multi-Core and Many-Core Processors (M. Sato, G. Fukazawa, K. Yoshinaga, Y. Tsujita, A. Hori, M. Namiki), In International Journal Advanced mputer Science (IJACSci), volume 3, 2013.

(2) Conference Papers

[3] Multithreaded Two-Phase I/O: Improving Collective MPI-IO Performance on a Lustre File System (Yuichi Tsujita, Kazumi Yoshinaga, Atsushi Hori, Mikiko Sato, Mitaro Namiki, Yutaka Ishikawa), In Proceedings of PDP2014, Turin, February 12-14, 2014, IEEE CS, 2014.

[4] 京での大量データの並列相関計算を支援するソフトウェアの提案 (吉永一美, 徳久淳師, 大野善之, 亀山豊久, 堀敦史, 城地保昌, 初井宇記, 石川裕), In 情報処理学会研究報告. [ハイパフォーマンスコンピューティング], 一般社団法人情報処理学会, volume 2013, 2013.

[5] メニーコア混在型並列計算機向け大域仮想アドレス空間モデル Multiple PVAS の提案 (深沢 豪, 佐藤 未来子, 吉永 一美, 辻田 祐一, 島田 明男, 堀 敦史, 並木 美太郎), In 情報処理学会第 141 回ハイパフォーマンスコンピューティング研究発表会, 一般社団法人情報処理学会, volume 2013, 2013.

[6] RDMA スケジューリングによる MPI 通信の高速化 (畑中正行, 堀敦史, 石川裕), In IPSJ

SIG Notes, Information Processing Society of Japan (IPSJ), volume 2013, 2013.

[7] メニーコア用 Agent プログラミング環境の提案 (Hori Atsuhi, Shimada Akio, Namiki Mitaro, Sato Mikiko, Fukazawa Go, Tsujita Yuishi, Ishikawa Yutaka), In IPSJ SIG Notes, Information Processing Society of Japan (IPSJ), volume 2013, 2013.

[8] ヘテロジニアス計算機上の OS 機能委譲機構 (佐伯 裕治, 清水 正明, 白沢 智輝, 中村 豪, 高木 将通, Balazs Gerofi, 思 敏, 石川 裕, 堀 敦史), Information Processing Society of Japan (IPSJ), volume 2013, 2013.

[9] メニーコア向けNUMA最適並列分散I/Oの予備検証 (小田和 友仁, 住元 真司, 堀 敦史, 石川 裕), Information Processing Society of Japan (IPSJ), volume 2013, 2013.

[10] 次世代高性能並列計算機のためのシステムソフトウェアスタック (石川 裕, 堀 敦史, Balazs Gerofi, 高木 将通, 島田 明男, 清水 正明, 佐伯 裕治, 白沢 智輝, 中村 豪, 住元 真司, 小田和 友仁), Information Processing Society of Japan (IPSJ), volume 2013, 2013.

[11] A Delegation Mechanism on Many-Core Oriented Hybrid Parallel Computers for Scalability of Communicators and Communications in MPI (Kazumi Yoshinaga, Yuichi Tsujita, Atsushi Hori, Mikiko Sato, Mitaro Namiki, Yutaka Ishikawa), In Proceedings of the 2013 21st Euromicro International Conference on Parallel, Distributed, and Network-Based Processing, IEEE Computer Society, 2013.

[12] Proposing a new task model towards many-core architecture (Akio Shimada, Balazs Gerofi, Atsushi Hori, Yutaka Ishikawa), In Proceedings of the First International Workshop on Many-core Embedded Systems, ACM, 2013.

[13] Optimization of MPI Persistent Communication (Masayuki Hatanaka, Atsushi Hori, Yutaka Ishikawa), In Proceedings of the 20th European MPI Users' Group Meeting, ACM, 2013.

[14] Partially Separated Page Tables for Efficient Operating System Assisted Hierarchical Memory Management on Heterogeneous Architectures (Balazs Gerofi, Akio Shimada, Atsushi Hori, Yutaka Ishikawa), In CCGRID, 2013.

(3) Patents and Deliverables

Open Source Software Packages (http://www.sys.aics.riken.jp/releasedsoftware/index.html)

[15] PRDMA (for the K computer)

[16] File Composition Library (for the K computer)

[17] GDB for McKernel

[18] PVAS, M-PVAS and Agent (for the x85 and Xeon Phi CPUs)

Programming Environment Research Team

1. Team members

Mitsuhisa Sato (Team Leader)

Hitoshi Murai (Research Scientist)

Miwako Tsuji (Research Scientist)

Masahiro Nakao (Postdoctoral Researcher)

Tomotake Nakamura (Research Associate)

Takenori Shimosaka (Research Associate)

Laurence Beaude (Research Trainee)

Swann Perarnau (Visiting Researcher, JSPS Research Fellow)

Masahiro Yasugi (Visiting Researcher)

Hitoshi Sakagami (Visiting Researcher)

Hiroaki Umeda (Visiting Researcher)

Horitz Helias (Visiting Researcher)

Susanne Kunkel (Visiting Researcher)

Tomoko Nakashima (Assistant (Concurrent))

2. Research Activities

The K computer system is a massively parallel system which has a huge number of processors connected by the high-speed network. In order to exploit full potential computing power to carry out advanced computational science, efficient parallel programming is required to coordinate these processors to perform scientific computing. We conducts researches and developments on parallel programming models and language to exploit full potentials of large-scale parallelism in the K computer and increase productivity of parallel programming.

In 2013FY, in order to archive these objectives above, we carried out the following researches:

1) We continued the development of XcalableMP(XMP) programming languages. XcalableMP is a directive-based language extension which allows users to develop parallel programs for distributed memory systems easily and to tune the performance by having minimal and simple notations. The specification has been designed by XcalableMP Specification Working Group (XMP Spec WG) which consists of members from academia and research labs to industries in Japan. We have been working with XMP Spec WG to improve the specification. In this year, we studied the optimization of reflect communication, and one-sided communication, and applications of climate applications using the XcalableMP. As an extension to exascale computing, we are designing a new programming model and developing its compiler for emerging accelerator clusters, by combining XcalableMP and

OpenACC. W have released the version 0.7.0 in November 2013, and deployed it to the K computer. We submitted the results to SC13 HPCC class 2 competition, and awarded "HPCC Class2 Award".

2) We have working for Japan-France project FP3C, "Framework and Programming for Post Petascale Computing", from 2012, and have been developed the integrated programming environment, called FP2C, of XcalableMP and YML which is developed by the French team. In this year, we carried out performance evaluation of FP2C programming using the K computer.
3) For large-scale parallel applications, we investigate a new parallel communication library to support the communication between a set of multiple processes in Multiple processes Multiple Data (MIMD)
4) For the research for performance tuning tools for large-scale scientific applications running on the K computer, we are supporting the Scalasca performance turning and analysis tool developed by JSC, Germany, on the K computer. We have deployed it on the K computer as our AICS-supported software.
5) Aiming to explore runtime technologies of post-petascale computing, we studied the performance of work-stealing on the K computer for dynamic distributed load balancing. In this year, we designed a new load balancing efficiency metric to evaluate the performance of work-stealing.
6) We conducted several collaborations on the performance evaluation with JSC, University of Tsukuba and other groups.

In addition to the research activities, we conduct promotion activities to disseminate our software. To promote XcalableMP as a means for parallelization of programs, we made the XcalableMP workshop, seminars or lectures as follows.

- XcalableMP workshop (Nov. 1)
- FOCUS seminar (July 16, Sep. 18, Dec. 18)
- Earth Simulator user meeting (Oct. 17)

The seminar or lecture consists of both classroom and hands-on learning

3. Research Results and Achievements

3.1. Development of XcalableMP compiler

We are developing Omni XcalableMP that is an open-source XcalableMP compiler, in cooperation with Tsukuba University, and released the version 0.7.0 in November 2013.

3.1.1 Optimization of Reflect communication in stencil computation

The key changes in this version are the improvements of stencil communications in performance and conformance to the language specification, which is related with XMP's shadow and reflect directives [1]. First, three methods of data transfer in stencil communication were implemented:

- Based on the MPI's derived datatype: Array elements on distribution boundary are transferred in a batch as a derived datatype. The performance depends on the implementation of MPI, but it is an advantage that it can be applied in any environment.
- Based on parallel packing/unpacking: Data is packed to a buffer with multithreading before communication and unpacked from a buffer. This can be effective in multicore environments.
- Based on RDMA of the K compute: Using the extended interface of RDMA available on the K computer, stencil communications can be implemented more efficiently than using MPI. Each contiguous block of array elements is put to the corresponding location in the stencil area on the neighbor node.

Users can select with an environment variables which method is to be used in their XcalableMP program.

Secondly, functions of the reflect directives are fully implemented for XMP/Fortran. The function includes:

- the width clause
- the periodic modifier
- the async clause

3.1.2 Evaluation of productivity and performance of XcalableMP: HPCC Class2

In order to evaluate productivity and performance of XcalableMP, we have implemented HPC Challenge (HPCC) benchmarks. The HPCC benchmarks are a set of benchmarks to evaluate multiple attributes of an HPC system. The HPCC benchmarks consist of RandomAccess, Fast Fourier Transform (FFT), High Performance Linpack (HPL), and STREAM. We have implemented them by using XcalableMP. In addition, we have implemented the Himeno Benchmark, which is a typical stencil application. Table 1 shows the source lines of code (SLOC) of our implementations. The SLOCs of XcalableMP are smaller than those of the reference implementations by using MPI.

Table 1: Source lines of code of HPCC and HIMENO benchmarks.

	HPL	RandomAccess	FFT†	STREAM	HIMENO
XcalableMP	306	250	70	66	137
Reference	8,800	938	101	329	380

†Only kernel implementation

All benchmarks were compiled by using the Omni XMP compiler 0.7.0-alpha. In order to evaluate the performances of these benchmarks, we used all compute nodes at a maximum on the K computer. For comparison, we also evaluated the some reference implementations. For HPL, we compared our performance with the theoretical performance. Fig. 1 shows the performance results. The performances of XcalableMP implementations are almost the same as those of the reference implementations.

Through these implementations and performance evaluations, we have revealed that XcalableMP has good productivity and performance. We have submitted the results to the SC13 HPC Challenge Benchmark Class2 Competition, and we have awarded the HPC Challenge Class 2 Award.

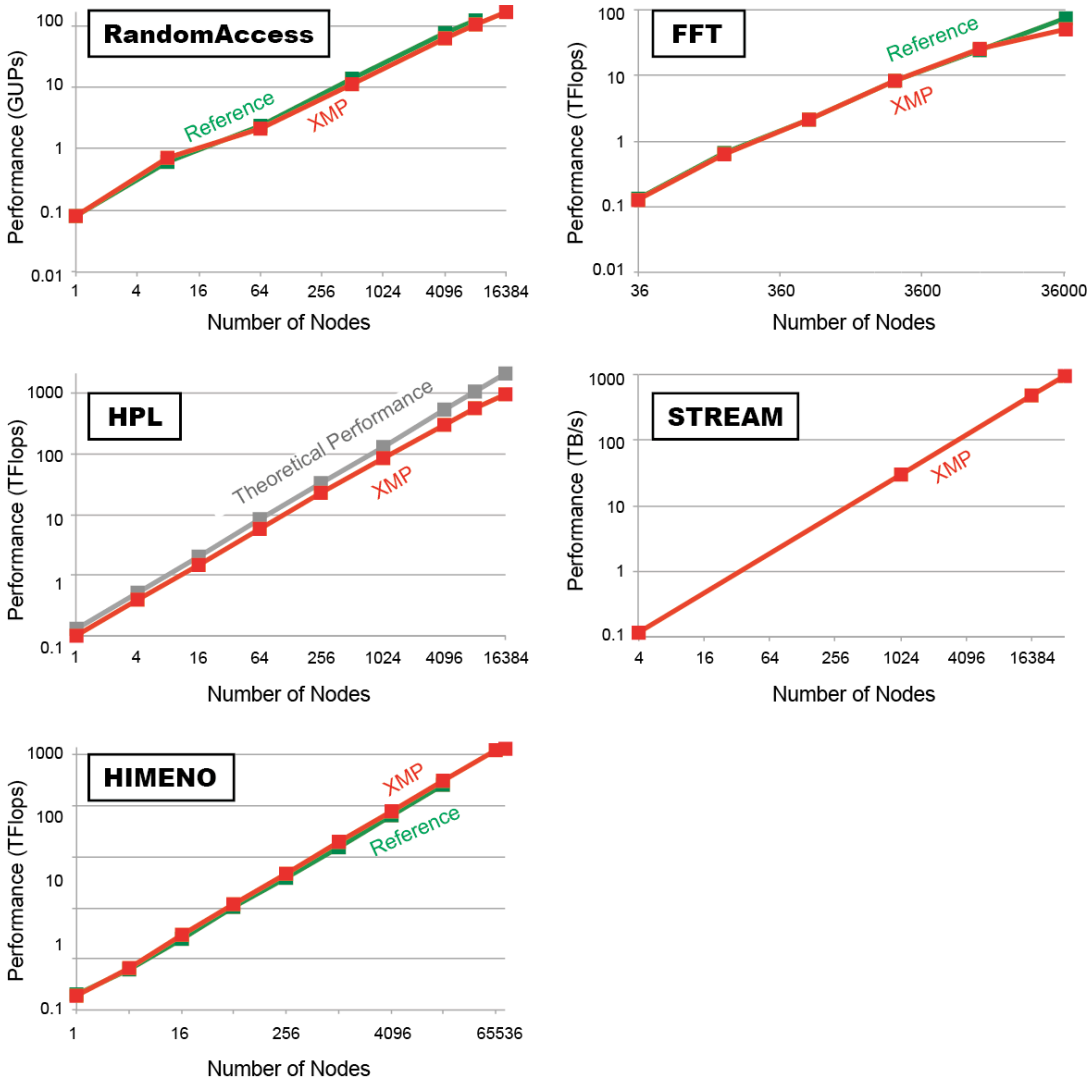


Fig 1. Performance results of HPCC benchmarks and HIMENO benchmark.

3.1.3 Evaluation of climate applications on the K computer

Exascale computing will enable us to predict a high-precision climate change by using very high-resolution model. In this study, we have ported following existing climate applications to the K computer and evaluated their performance.

- CGPOP Miniapp (CGPOP) : Mini application of global ocean modeling.
- NICAM : Global cloud resolving model.
- CICE : Sea ice model.

In order to improve productivity, we have used coarray syntax provided by XcalableMP for the porting. This study is a part of "G8 ESC - Enabling Climate Simulations at Extreme Scale," project with partners of US, France, Germany, Spain, and Canada.

The CGPOP needs a reduction operation by all compute nodes. We have implemented to use

hardware support of the reduction operation provided by the K computer. Next, the all applications need a sleeve exchange operation. We have implemented the exchange operation by using RDMA API provided by the K computer. This operation is supposed to use the coarray syntax. Finally, we have added OpenMP directives in CGPOP to perform thread-parallelization. Fig. 2 shows the performance results. We achieve 84% speed up in CGPOP, and 7% speed up in NICAM, and 15% speed up in CICE. In addition, by using coarray syntax, the codes of them are simpler than those of original ones.

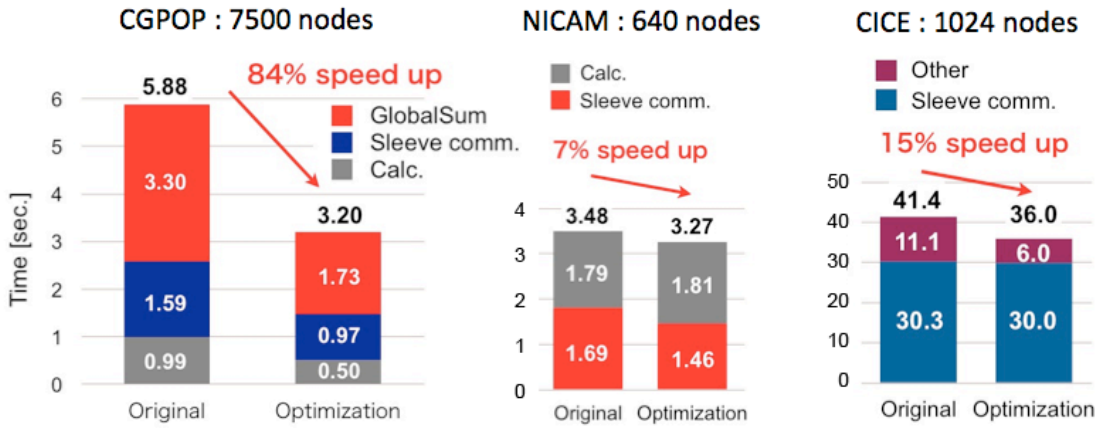


Fig 2. Performance results of Climate applications.

3.1.2 Extensions for Tightly Coupled Accelerators

We are designing a new programming model and developing its compiler for emerging accelerator clusters. Specifically, out target is accelerator clusters that are capable of direct communication between two accelerator devices on different nodes, called Tightly Coupled Accelerators (TCA). TCA is a next-generation device for communication between accelerators. In order to improve productivity of applications using TCA and accelerators, we have developed a new programming model as an extension of XcalableMP.

Our basic idea is combining XcalableMP and OpenACC. OpenACC is a directive-based API for offloading programs written in C, C++ and Fortran programs from a host CPU to an attached accelerator device. In our approach, XcalableMP directives are used to specify global-view-based parallel processing among nodes and OpenACC ones to control accelerator devices. The function of direct communication between accelerators is also provided as an extension to XcalableMP. This new programming model can significantly improve productivity in writing programs for accelerator clusters. Fig. 3 shows an example of the proposed programming model. Programmer only adds XcalableMP directives and OpenACC directives, and programmer can develop applications using TCA and accelerators.

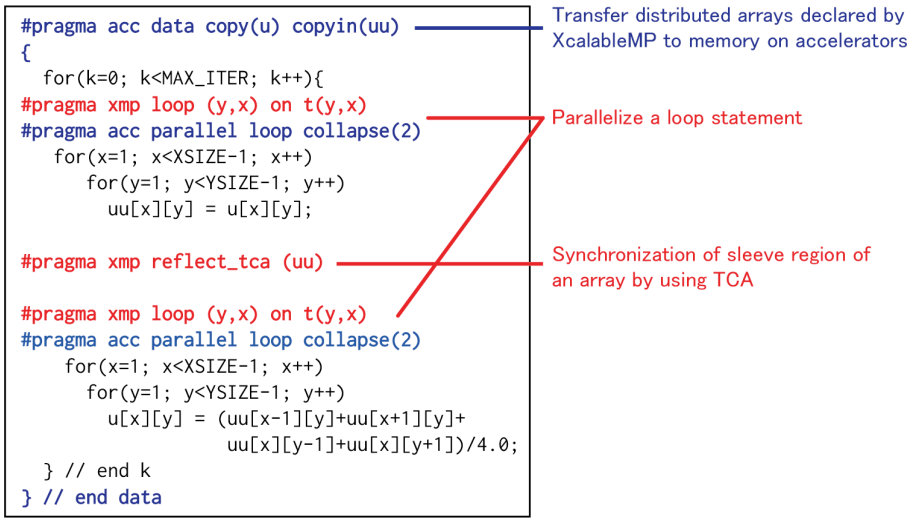


Fig 3. Example of the proposed programming model for TCA.

We have evaluated its performance on HA-PACS/TCA cluster, which is the demonstration system with TCA. As a result, the performance of the proposed programming model is almost the same as that of the application that directly uses native APIs of TCA.

This research is supported by CREST, JST.

3.2 FP3C Project & FP2C Software

FP3C (Framework and Programming for Post Petascale Computing) project is a French-Japanese collaborative research project involving INRIA, CNRS, CEA, and Maison de la Simulation (in France) and University of Tsukuba, University of Tokyo, Institute of Technology of Tokyo, the University of Kyoto and RIKEN AICS (in Japan). The project started on September 1st, 2010, and continued until March 31th, 2014. The aim of the project was to establish software technologies, to propose languages and programming models to explore extreme performance computing beyond petascale computing.

It is expected that post-petascale systems will be a huge, heterogeneous and highly hierarchical architecture with nodes of general processing cores and accelerator cores. For the programming models currently considered, for example the hybrid programming model of MPI+OpenMP, it would be sometimes difficult to exploit such systems efficiently. It would be essential to use multiple programming methodologies across multiple architectural levels. Based on this new programming model, we have developed the FP2C (Framework for Post-Petascale Computing) software to develop and execute applications on large, hierarchical and heterogeneous systems.

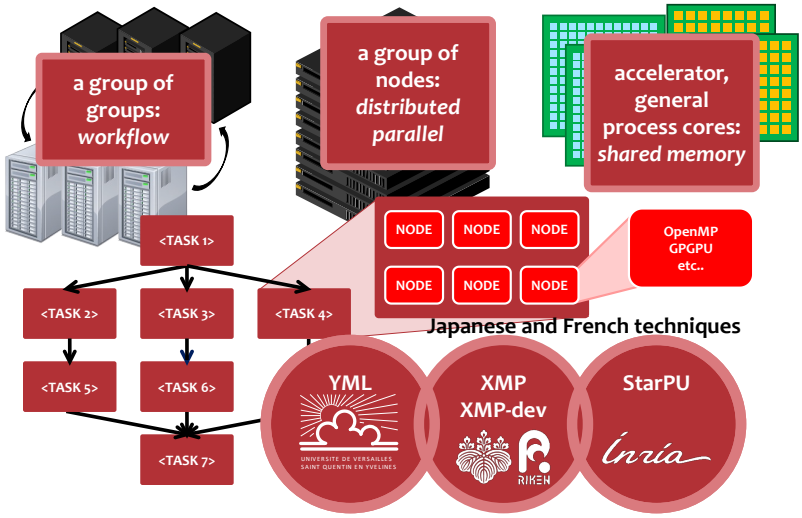


Fig 4. Overview of FP2C software.

Fig. 4 shows the overview of FP2C, which consists of workflow (supported by YML), distributed parallel programming model (supported by XMP) and shared memory/GPPGU programming model (supported by XMP-dev/StarPU). Within a group of tightly connected nodes, we adopt distributed programming model, and within a node composed of processing/accelerator cores, we adopt shared-memory/GPGPU programming model. These hybrid distributed parallel programs are considered to be tasks of a workflow. Therefore, between the groups of node, there is a workflow programing model, to manage and control these tasks. In order to develop FP2C software to realize the hierarchical programming model, we combine many Japanese and French techniques described above during this collaborative project.

One advantage of FP2C over the traditional workflow is that we can extend tasks by introducing distribute parallel programming model into its tasks to speed-up the tasks and overall application. Another advantage of FP2C over the traditional distributed parallel programming model is that we can divide a large parallel program into several moderate sub-programs to avoid the communication cost in the large program. Additionally, we can construct a complicated program easily by combining existing parallel programs and parallel libraries (such as Scalapack) based on the workflow paradigm.

We have performed experiments on the K-computer with Block-Gauss-Jordan problem in order to investigate the different levels of hierarchical parallelisms. Therefore, in our experiments, while the matrix size is fixed, the number of blocks is varied. Also, while the total number of processors for a workflow application is fixed, the number of processers for each task is varied. As shown in the Fig. 5, the best result has been obtained from the mixture of different programming paradigms which realized based on our framework.

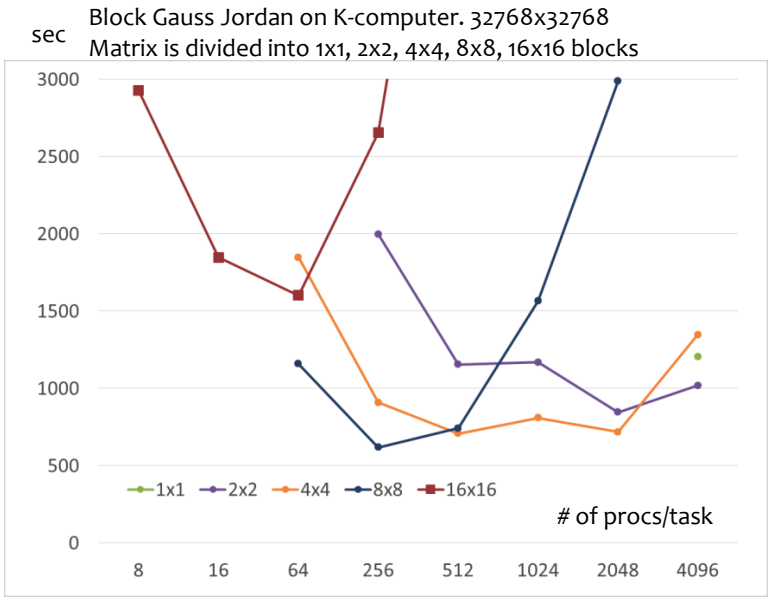


Fig 5. Performance of Block Gauss Jordan Method using FP2C on the K computer.

We have also implemented multiple implicitly restarted Arnoldi methods (MIRAM) with FP2C. The MIRAM is an eigen-solvers investigated by another group of the FP3C project. The MIRAM, which invokes two or more interacting restarted Arnoldi solvers, was particularly designed to be suited for environments that combine different parallel programming paradigms, i.e. coarse and fine grain parallelisms. Inside each solver, fine grain parallelism such as distributed parallel model is realized by XMP or MPI. The solvers communicate each other based on coarse grain parallelism realized by YML. The MIRAM for dense and sparse matrices are implemented with YML, XMP, MPI, and external libraries such as Petsc, Slepc, and PARPACK.

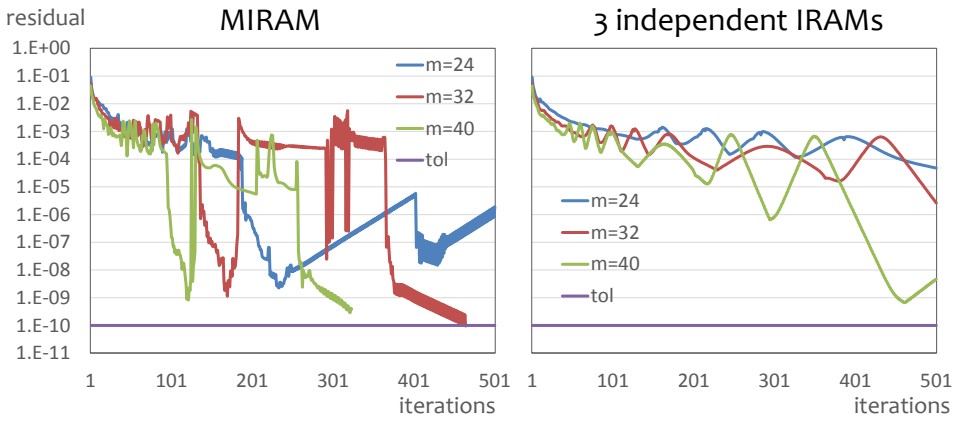


Fig 6. Performance of MIRAM using FP2C on the K computer.

Fig. 6 shows the experimental result of MIRAM for the sparse matrix called "Schenk/nlpkkt240" (Rows x Colmns = 27,993,600 x 27,993,600, 760,648,352 non-zero elements) provided by UF Sparse Matrix Collection. According to the evaluation on the K computer, 2 different kinds of speedup based on 2 different parallel models have been observed:

- Speedup convergence by the interactions of multiple solvers based on the cause grain parallelism
- Speedup each iteration based on the fine grain parallelism.

3.3 Communication Library between Multiple Sets of MPI Processes for MPMD model

An MPMD programming model is widely used as a master-worker program or a coupling program for multiple physical models. Recent high-end parallel computers have more than several thousand nodes. In order to utilize the parallel computers for an MPMD model, we proposed the communication library MPMPI between different multiple sets of MPI processes for the MPMD model.

We designed the basic MPMPI function MPMPI_Send and MPMPI_Recv. In order to effectively develop the interface specification of MPMPI_Send/Recv, we referred to the concept of some basic MPI functions. One of the features of the MPMPI functions is the exchange of distributed data between sets of processes having different shapes or different distribution methods. We also designed the MPMPI interfaces for the XcalableMP PGAS language. MPMPI_Send and MPMPI_Recv have been currently implemented in C language and the MPI_Send/Recv functions. They currently support one and two dimensional block distribution methods.

Fig. 7 shows the performances of the master-worker program with the Block Gauss Jordan algorithm using our library. We programs are implemented in XcalableMP/C (XMP/C). An experimental environment is the K computer system. Fig.7 shows the basic performance of MPMPI_Send/Recv. We assume that a whole matrix is stored in multiple main memories. For matrix products on each process of worker programs in the BGJ program, we utilized the thread parallelized LAPACK and the BLAS library provided by the K computer system. The sizes (n × n) of the input matrix A in the BGJ program are 16384 × 16384, 32768 × 32768 and 65536 × 65536. They are distributed onto 32 × 32 nodes in the master program. The numbers of nodes that one MPMPI communication uses are 2×2, 4×4, 8×8, 16×16 nodes.

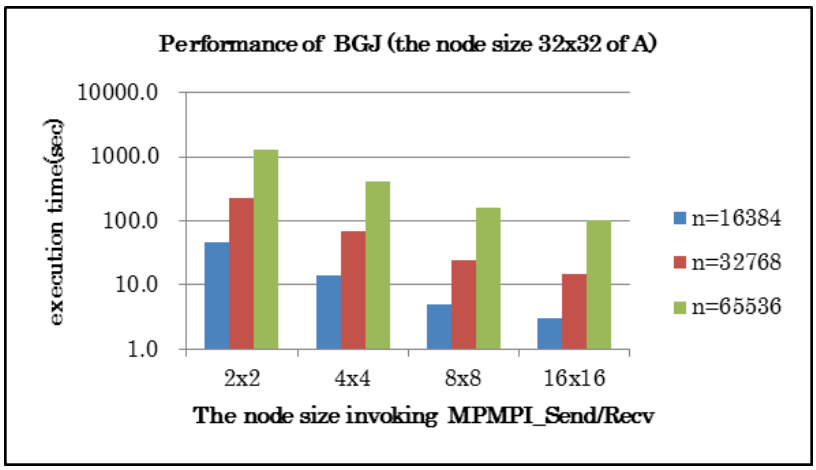


Fig 7. Performance of the master-worker program with Block Gauss Jordan algorithm using MPMPI

We found that the elapsed times of the master-worker program decrease as the numbers of nodes that one MPMPI communication uses increases. The percentages of the MPMPI communications are less than 10% for all cases.

3.4 Performance Study and Optimization of Distributed Load Balancing on the K computer

Distributing computations, in particular irregular ones, at such scale requires increasingly complex and dynamic load balancing systems. Work stealing is a provably efficient scheduling algorithm for such distributed, dynamic load balancing requirements. It is becoming increasingly popular, both for shared memory systems (intra-node load balancing) and in distributed settings (inter-node load balancing). We studied the performance of work-stealing on the K Computer in regards to a previously overlooked issue in High Performance Computing settings: the impact of large scale latencies. Using the publicly available, MPI-based implementation of the Unbalanced Tree Search (UTS) benchmark, we evaluated the performance of work stealing at the scale of several thousands compute nodes.

This implementation of UTS follows the general structure of any work stealing application. When work is available, a process retrieves a node from its stack. This node's data is then used to compute its children, which are pushed into the stack. If no work is available, a victim process is selected, and work is fetched from its stack. This process continues until all work is exhausted. Such condition is detected by a token-ring distributed termination algorithm. Fig. 8 presents the speedup of this same benchmark between 1024 and 8192 MPI Processes, for 3 process allocations (1 rank per node, 8 ranks per node in round robin, 8 consecutive ranks per node). This figure demonstrates that this UTS implementation does not scale past 2048 nodes. Additionally, it appears that the benchmark performance is severely impacted by the way in

which processes are distributed among compute nodes. In particular, allocating successive ranks to different compute nodes results in the worse performance observed.

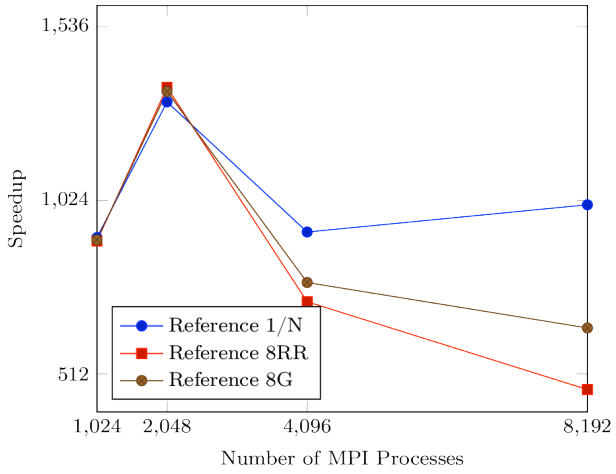


Fig 8. Speedup of the reference MPI work stealing implementation in the K computer.

To explain those results, we designed a new load balancing efficiency metric. The role of a dynamic load balancing scheme is to maximize the amount of processes having work at any given time. Thus, if a problem is comprised of enough work items, the state of an application should roughly be separated in three phases: the starting phase where work is distributed to all processes, the finishing phase during which work becomes scarce and the number of active processes decreases and the middle phase for which most processes are processing work. If work generation is irregular, as with UTS, balancing is also needed during the middle phase, but an efficient framework should be able to maintain a reasonable amount of processes busy. This intuition drives the definition of our performance metric. If one was to trace the active and idle phases of each process participating in the computation, it should be possible post-mortem to determine the number of active processes at any time during execution of the application.

We define here active phases as periods of time during which a process's stack contains work. Thus, in the chosen UTS implementation, all the time where a process is generating new nodes or handling MPI operations in between, (responding to steal requests for example) count as active. Similarly, a process is inactive if it does not have work locally. It should be noted that with such definition, most types of load balancing operations can be counted in either type of phase. Assuming there exists a trace of all processes indicating the time of each transition from one type of phase to the other, with the starting time of the application as t = 0, we now define the following metrics.

First, let workers(t) be the number of processes in an active phase at time t. From this number

we derive the maximum number of workers at any given time during execution Wmax and an occupancy ratio O(t) = workers(t)/N, N being the number of processes executing the application. Second, let the starting latency be SL(x) = min(t,O(t)=x) /T, with T the total execution time of the application. This measure computes, for a given occupancy ratio, the first time it was exceeded during execution and represent it as a ratio of the total execution. Similarly, we define the ending latency as EL(x) = (T –max(t,O(t)=x))/T . Intuitively, the starting latency gives us the speed, relative to the total execution time of the application, at which a number of processes becomes active. The ending latency reflects a similar idea: how far away in the execution the framework is able to maintain a number of processes active. Fig. 9 shows the results of starting and ending latencies for an execution of the reference implementation with 8192 MPI processes, 1 process per node in the K computer. Data is limited to latencies lower than 10%.

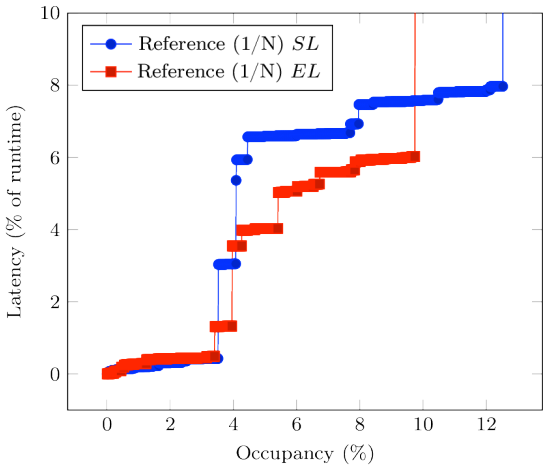


Fig 9. Starting and Ending latencies in the K computer.

On the K computer, latencies between nodes in the same blade are lower than inside the cube or across racks. Furthermore, the number of compute nodes inside a rack (only 96) means that an allocation of 8192 nodes can easily span across more than 80 racks, and in practice we observed that a communication between two processes can go through more than 10 hops.

To reflect these variations in response times for a steal, we designed a random selection strategy using a biased distribution. The idea is the following: while preserving the ability to steal any process, weight the probability of one process stealing another by the distance between those two. The farther a process is, the lower the probability of being chosen. As the Fujitsu MPI implementation provide extensions to query the 6D coordinates in the Tofu network of any MPI rank, we used the Euclidean distance between nodes to weight the probability. Fig. 10 shows the results improved by this approach, as indicated as "Tofu".

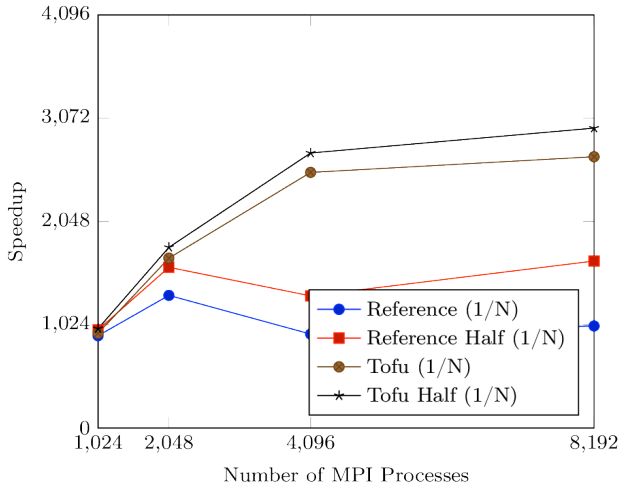


Fig 10. Speedup of the MPI work stealing implementations by using topology of Tofu network.

4. Schedule and Future Plan

One of important archivement of this year was that our XcalableMP submission was awarded HPCC Class2 Awards to be given for high productivity and performance. To extend this acheivement, the important action is to disseminate our XcalableMP to applications users. Actually, in this year, we organized several schools and hands-on, workshop with potential users. We will continue these promotion activities for the next year while we will study more optimization technique of XcalableMP compiler to improve the performance. As a research agenda especially for the K computer, we will contribute the scalability of large-scale applications for the K computer.

For the performance turning tools, we have been supporting Scalasca for the K computer. The next step will be to integrate with XcalableMP to make the performance tuning process easily. We have already done this partially for C, and will extend it to real large applications written in Fortran for more integrated programming environment for larege-scale parallel computing. Through these case studies, we will extend it for valuable performance analysis in the K computer.

The programming models for post-petascale will be investigated, including programming models and runtime techniques to support dynamic load balancing in large-scale parallel programs, and parallel programing supports for new communication devices, TCA, in advanced GPU clusters.

5. Publication, Presentation and Deliverables

(1) Conference Papers

[1] Hitoshi Murai, Mitsuhisa Sato. "An Efficient Implementation of Stencil Communication for the XcalableMP PGAS Parallel Programming Language", 7th International Conference on PGAS Programming Models, Edinburgh UK, Oct. 2013.

[2] Masahiro Nakao, Hitoshi Murai, Takenori Shimosaka, and Mitsuhisa Sato. "Productivity and Performance of the HPC Challenge Benchmarks with the XcalableMP PGAS Language", 7th International Conference on PGAS Programming Models, Edinburgh UK, Oct. 2013.

[3] Serge Petiton, Mitsuhisa Sato, Nahid Emad, Christophe Calvin, Miwako Tsuji and Makarem Dandouna, Multi-level programming Paradigm for Extreme Computing, Joint International Conference on Supercomputing in Nuclear Applications + Monte Carlo,2013.10.27-31, Paris France.

[4] Miwako Tsuji, Mitsuhisa Sato, Maxime Hugues and Serge Petiton, Multiple-SPMD Programming Environment based on PGAS and Workflow toward Post-Petascale Computing, Proceedings of the 2013 International Conference on Parallel Processing (ICPP-2013), 480--485,2013.10.01-04, Ecole Normale Superieure de Lyon Lyon France.

[5] Miwako Tsuji, Makarem Dandouna and Nahid Emad,Multi level parallelism of Multiple implicitly/explicitly restarted Arnoldi methods for post-petascale computing,Proceedings of the 8th IEEE International Conference on P2P Parallel Grid Cloud and Internet Computing (3PGCIC-2013),158--165,2013.10.28-30,University of Technology of Compiegne Compiegne France.

[not refereed, in Japanese]

[6] Masahiro Nakao, Hitoshi Murai, Takenori Shimosaka, Akihiro Tabuchi, Yuetsu Kodama, Taisuke Boku, Mitsuhisa Sato, "Extension of XcalableMP for Tightly Coupled Accelerators", IPSJ SIG Technical Report, Mar. 2013 (in Japanese).

[7] Masahiro Nakao, Mitsuhisa Sato, "Implementation of NICAM by using PGAS model language on the K computer", Vol.2013-HPC-140, pp.1-5 Aug. 2013 (in Japanese).

[8] Masahiro Nakao, Mitsuhisa Sato, "Performance measurement of CGPOP Mini-application on the K computer", IPSJ SIG Technical Report, May 2013 (in Japanese).

[9] T. Shimosaka, M. Sato, T. Boku, W. Tang. Evaluation of the nuclear fusion simulation code GTC-P on the K computer. IPSJ SIG Technical Report, May. 2013 (in Japanese).

(2) Invited Talks

[10] Mitsuhisa Sato, Issues for Exascale Accelerated Computing - system architecture and programming, 7th Int'l. Conf. on PGAS Programming Models.

(3) Posters and Presentations

[11] Masahiro Nakao, Hitoshi Murai Takenori Shimosaka Mitsuhisa Sato. "XcalableMP for Productivity and Performance in HPC Challenge Award Competition Class 2", SC13 The 2013 HPC Challenge Awards BoF, Denver, Colorado, USA, Nov., 2013.

[12] Masahiro Nakao, "Performance and productivity of XcalableMP", 5th cross-disciplinary symposium of computational science – development, assimilation, and construction of new knowledge", Nov. 2013 (in Japanese).

[13] Nahid Emad, Leroy Drummond, Miwako Tsuji and Makarem Dandouna, Tuning Asynchronous Co-Methods for Large-scale Eigenvalue Calculations 16th SIAM Conference on Parallel Processing for Scientific Computing, 2014.02.18--21, Portland Marriott Downtown Waterfront Portland OR USA, 2014.

[14] T. Shimosaka, H. Murai and M. Sato, A communication library between multiple sets of MPI processes for a MPMD model, pp. 147–148(poster), EuroMPI2013, 2013.

[15] Swann Perarnau, Mitsuhisa Sato, Weighted Distribution for Random Victim Selection in Distributed Work Stealing, HPC in Asia Workshop, International Supercomputing Conference (ISC), Leipzig Germany, June 2013.

(4) Patents and Deliverables

[16] Omni XcalableMP compiler ver. 0.7for the K computer (registered as AICS-supported software)

[17] Scalasca performance analysis tool for the K computer (registered as AICS-supported software)

Processor Research Team

1. Team Members

Makoto Taiji (Team Leader)
Yousuke Ohno (Senior Research Scientist)
Noriaki Okimoto (Senior Research Scientist)
Gentaro Morimoto (Research Scientist)
Takao Otsuka (Research Scientist)
Yoshinori Hirano (Research Scientist)
Tomoki Kobori (Postdoctoral Researcher)
Yohei Koyama (Postdoctoral Researcher)
Aki Hasegawa (Research Associate)
Yumie Ohyama (Assistant)

2. Research Activities

The aim of the processor research team is to create a future basis of high-performance processors for scientific simulations, as well as to explore the processor performance of the K computer.

In future high performance computing, we have to tackle with millions or more parallel operation units to extend the performance. However, many applications require acceleration while keeping the problem size, i. e. the strong scaling, and they can often be parallelized up to thousands of core, not to millions. To achieve better strong scaling, we have to decrease the cost of parallelization by improving the latency in everywhere – network, main memory, and processors. For this, we will try to develop the platform of System-on-Chip (SoC) based accelerators. It consists of general-purpose processor cores, memories, network units and computing accelerators on the single chip. By such integration we aim to achieve the ultimate performance for selected applications.

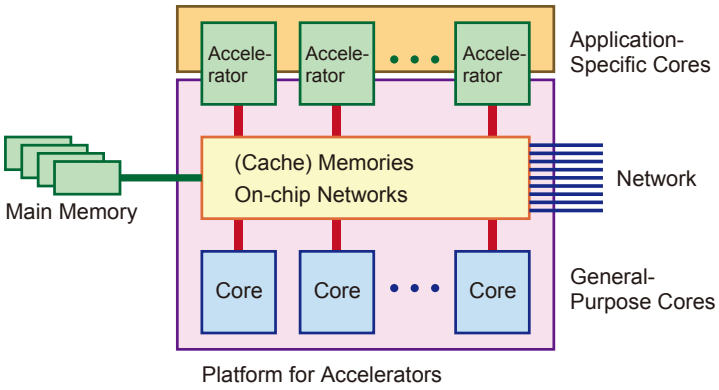


Fig. 1. Diagram of platform for accelerators.

In addition to the researches on future computing platform, we will contribute to accelerate the application performance on the K computer. The processor of K computer, SPARC64 VIIIfx, has several special features for high-performance computing called VISIMPACT and HPC-ACE. We will explore to extract its power for several applications based on our experience on the processor architecture.

3. Research Results and Achievements

3.1. Platform of accelerators

In this year we evaluated the MDGRAPE-4 SoC in RIKEN QBiC (Quantitative Biology Center) using the test board of the MDGRAPE-4 system. We have confirmed the basic operation of SoC. We are porting GROMACS software for the MDGRAPE-4 system with Prof. Lindahl, Stockholm University.

From the viewpoint of the platform of SoC based accelerator, we can use as the MDGRAPE-4 SoC as the basis. It has 65 general-purpose (GP) processor cores, 64 dedicated pipelines for molecular dynamics force calculation, main memories, and network units for 3-dimensional torus network. By replacing the dedicated pipelines we can use the design as the platform of accelerators. The operation frequencies of the dedicated pipelines and the GP cores are 0.8 GHz and 0.6 GHz, respectively. For the inter-process synchronization, the queue system in the GP core is used. The pipeline units, the GP cores, and the network units exchange message with the control GP core, which takes control of a whole calculation. The SoC also contains a shared memory unit of 1.8MB. The size of SoC is 15.6×15.6 mm^2, and is fabricated by the Hitachi HDL4S 40nm bulk CMOS technology. Its pipelines can evaluate 51.2G interactions/sec, which is equivalent to 2.56 Tflops performance when we count the calculation cost of a nonbond force and a potential as 50 flop.

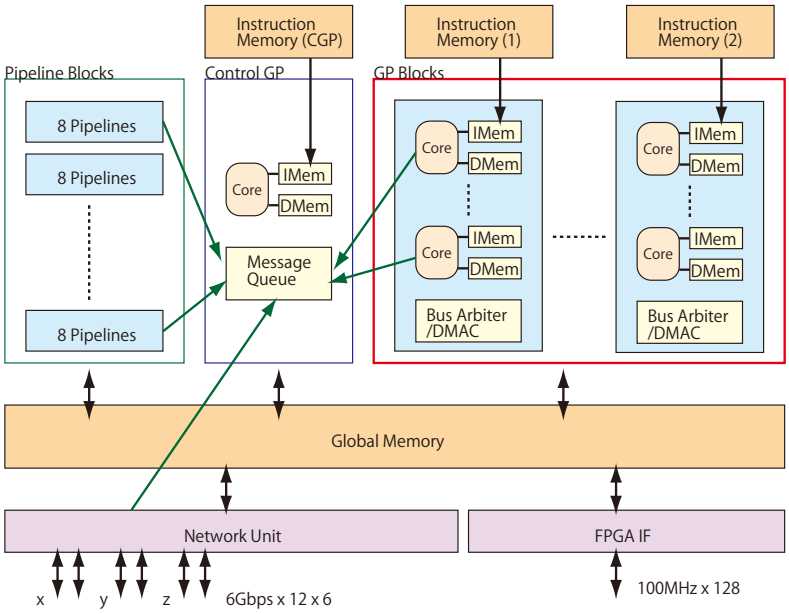


Fig. 2. Block diagram of MDGRAPE-4 SoC.

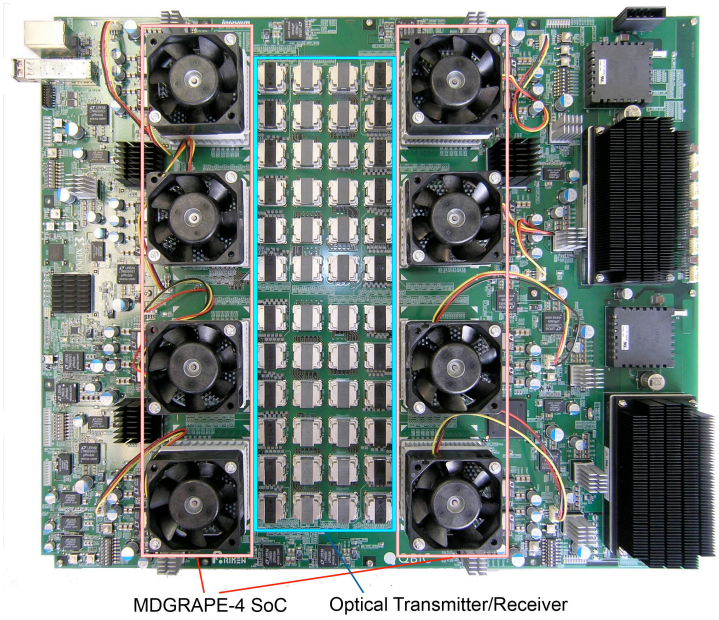


Fig. 3. MDGRAPE-4 system board.

3.2 Application Optimization on K computer

For application optimization we have optimized the molecular dynamics core code.

4. Schedule and Future Plan

In the next year, we will finish the MDGRAPE-4 System in RIKEN QBiC. In future, we will continue to implement the part of the MDGRAPE-4 SoC as the platform of accelerators. We will also

develop network-on-chip architecture for specific purposes like machine learning/ neural network. We will continue the optimization of MD core and the other codes for the K computer. We will also start the drug design and medical application of high-performance computing with Prof. Yasushi Okuno, senior visiting scientist.

5. Publication, Presentation and Deliverables

(1) Invited Talks

[1] Makoto Taiji, "MDGRAPE-4: a special-purpose computer system for molecular dynamics simulations," Royal Society Kavli Seminar on "Multiscale systems: linking quantum chemistry, molecular dynamics, and microfluidic hydrodynamics", Chicheley Hall, Buckinghamshire, UK (2013/7/22-23).

[2] Makoto Taiji, "MDGRAPE-4: a special-purpose computer system for molecular dynamics simulations," Plenary Lecture, Joint Workshop on Bio-inspired Engineering and Bio-supercomputing, Chiba University, Chiba, Japan (2014/3/3-4).

Large-scale Parallel Numerical Computing Technology Research Team

1. Team members

Toshiyuki Imamura (Team Leader)

Takeshi Fukaya (Post Doctoral Researcher)

Yusuke Hirota (Post Doctoral Researcher)

Yoshiharu Ohi (Post Doctoral Researcher)

Daisuke Takahashi (Senior Visiting Researcher)

Franz Franchetti (Visiting Researcher)

Yoshio Okamoto (Visiting Researcher)

Yukiko Hayakawa (Assistant)

2. Research Activities

The Large-scale Parallel Numerical Computing Technology Research Team conducts research and development of a large-scale, highly parallel and high performance numerical software library for K computer. Simulation programs require various numerical techniques to solve linear systems, eigenvalue problems, fast Fourier transforms, and non-linear equations. In order to take advantage of the full potential of K computer, we must select pertinent algorithms and develop a numerical software library based on the concepts of high parallelism, high performance, high precision, resiliency, and scalability.

Our primary mission of this project is to develop a highly parallelized and scalable numerical library on the K computer system, namely KMATHLIB. It comprises several components such as for solving

1) System of linear equations,
2) Eigenvalue problems,
3) Singular value decomposition,
4) Fast Fourier transforms, and
5) Nonlinear equations.

The K-specific topics are also our challenging works as follows;

a) Tofu interconnect,
b) Parallel I/O,
c) Fault detection (soft-error), and
d) Higher accuracy computing.

We are going to complete this project through close collaboration among computational science (simulation), computer science (hardware and software) and numerical mathematics. Our final goal is to establish a fundamental technique to develop numerical software libraries

for next generation supercomputer systems based on strong cooperation within AICS.

3. Research Results and Achievements

In this report, we focus on our three projects, 1) development of KMATHLIB, 2) development of EigenExa, and 3) investigation of the FDTD related method. Other activities by each researcher and collaborative works with other AICS teams are summarized in the last two sections, future plans and the publication list.

3.1. KMATHLIB Project

1. **Development of the KMATHLIB for the integration of OSS packages**

Since FY2012-2013, we have developed an integration framework KMATHLIB for number of numerical libraries installed on K computer. KMATHLIB supports a wide range of spectral of a lot numerical libraries, and KMATHLIB-API covers the resource usage from hundred to ten-thousand nodes or up to the whole system.

The schematic of KMATHLIB is depicted in Figure 1. KMATHLIB-API is on the top layer and is accessed by users directly. By taking account of KMATHLIB, we can plug-in favorite OSS like the bottom part of Figure 1. KMATHLIB-API can conceal the differences of API's and data structures, etc.

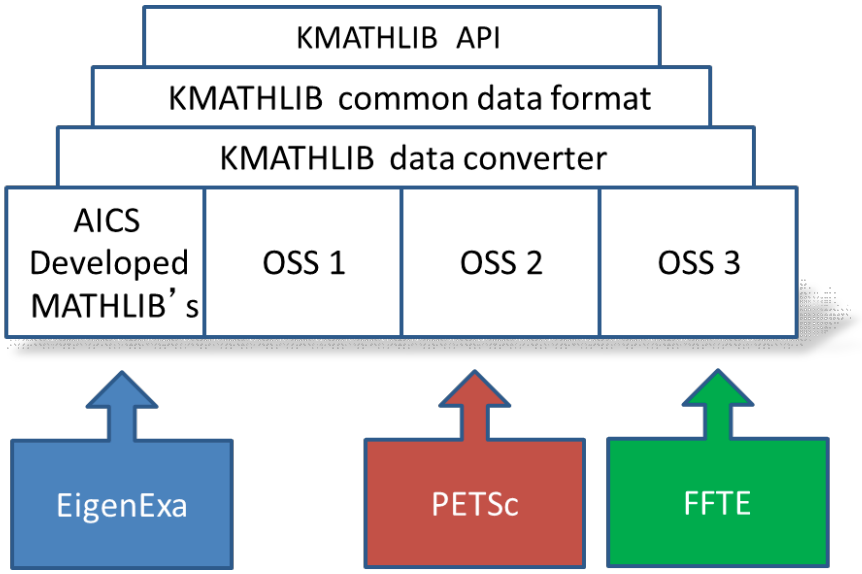


Figure 1. The structure of the KMATHLIB package.

Example of KMATHLIB-API is shown in Figure 2. KMATHLIB-API adopts a modern API style of the standard numerical libraries, like PETSc and FFTW. In order to use the numerical solver plugged in the KMATHLIB package, user needs to proceed four steps.

1. First, the user initiates KMATHLIB.
2. Create a handle of each solver. The handle is bound with several attributes about underlying data and options of the solver function to be called.
3. Then, the user invokes a solver function associated with the handle.
4. Finally, the finalization step must be done before the end of the program.

We have successfully integrated the standard numerical libraries such as LAPACK, ScaLAPACK, EigenExa, PETSc, FFTW, FFTE, and SSL II into the KMATHLIB package.

```
program xxx
use kmath_ls
Vec     x, b
Mat     A
KLS     kls

call Kmath_Initialize( )
call Kmath_LSCreate( MPI_COMM_WORLD, kls, ierr)

call Kmath_LSSolve( kls, A, b, x, ierr)

call Kmath_LSDestroy(kls, ierr)

end program
```

Figure 2. Example code of the KMATHLIB linear solver.

2. Enhancement of the KMATHLIB numerical libraries

Since FY2012-2013, we also have examined the parallel performance of the standard parallel OSS, and we have concluded that most of OSS does not scale on a large number of processors. We decided to develop and enhance the performance of ported OSS. In this report, we present two notable results of KMATH_RANDOM (random number generator) and newly proposed Divide and Conquer method for GEPBs.

a) Enhancement of the KMATH_RANDOM library

In FY2012-2013, we parallelized and integrated an open source real random number generator dSFMT into the KMATHLIB framework, namely KMATH_RANDOM. To support it

on K computer, we modified KMATH_RANDOM in FY2013-2014 so that each MPI process restarts to generate real random numbers independently. We have evaluated the KMATH_RANDOM library on K computer. Figure 3 shows the strong scaling behavior of the generator function which successively yields one billion random numbers. Although KMATH_RANDOM performs well, it scales down slightly when the number of nodes is large.

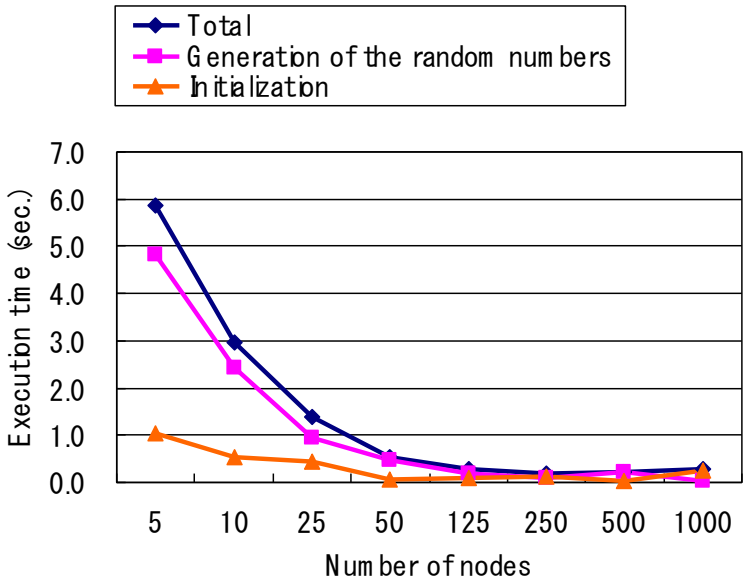


Figure 3. Strong scaling performance of KMATH_RANDOM on K computer.

b) New computational scheme by Divide and Conquer method for GEPBs

As a part of the KMATHLIB project, we have carried out basic research on a development of a solver for generalized eigenvalue problems of banded matrices (GEPBs)

$$A\boldsymbol{w} = \lambda B\boldsymbol{w}.$$

Here, A and B are N-by-N symmetric band matrices and B is positive definite. GEPBs often appear in quantum chemistry and the numerical solver of GEPBs can be used as a part of the solution method for dense symmetric definite GEPs. The faster performance of the solver for GEPB is strongly required. Rough analysis, however, reveals poor parallel performance of the conventional methods (e.g. parallelized versions of DSBGV and DSBGVD in LAPACK). We have proposed an alternative divide and conquer method for GEPBs which is based on the Elsner's idea (1997). The method has advantages that its FLOPS count is smaller than the conventional method and the most of the operations can be parallelized efficiently. Figure 4 shows the residuals $||AW - BW\Lambda||_F / ||A||_F$ obtained by the conventional solver (DSBGV) and a prototype of the proposed method. Here, $W = [\boldsymbol{w}_1, \boldsymbol{w}_2,$

…, $\boldsymbol{w}_N$], Λ = diag(λ_1, λ_2, …, λ_N), and (λ_i, $\boldsymbol{w}_i$) refers to the *i*-th eigenpair. We confirmed that the accuracy of the proposed is comparable to or better than the conventional method.

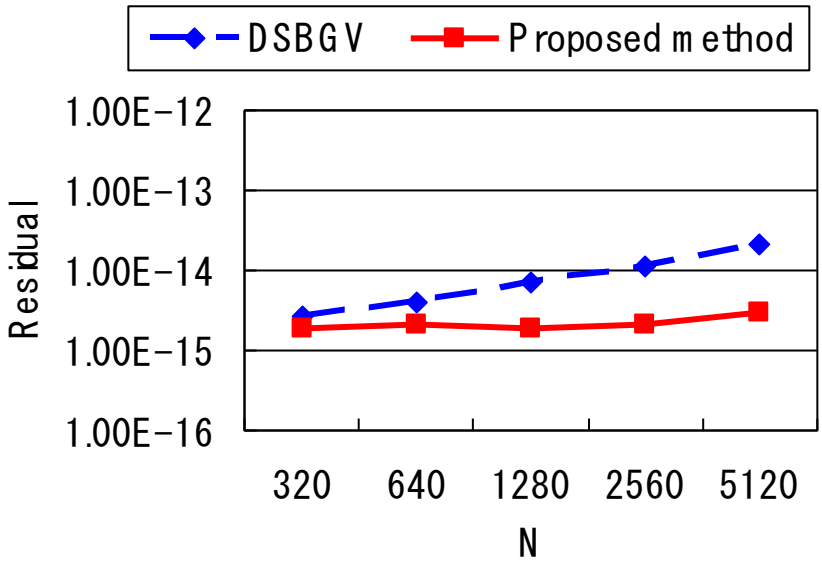


Figure 4. Accuracy test of DSBGV and the implementation of the proposed method.

3.2 EigenExa Project

The EigenExa Project is basically a collaborative work between Prof. Yusaku Yamamoto (formerly Kobe University, presently the University of Electro Communications) granted from 'Development of System Software Technologies for post-Peta Scale High Performance Computing' by JST CREST. We conduct mainly a part of the development of a high performance parallel dense eigenvalue solver, namely EigenExa.

1. Implementation of a Parallel solver

In a last Annual report for FY2012-2013, we reported the progress of this project and the status of the Eigen-K library. This FY2013-2014, the first version of the EigenExa library was released on August 2013 as a successor of Eigen-K. User can download EigenExa from the URL, http://www.aics.riken.jp/labs/lpnctrt/EigenExa_e.html.

From the same URL, we can refer to the poster (Figure 5) which was presented at International Workshop EPASA2014. Figure 5 illustrates the latest performance report and our outstanding achievement of world largest scale eigenvalue computation on K computer.

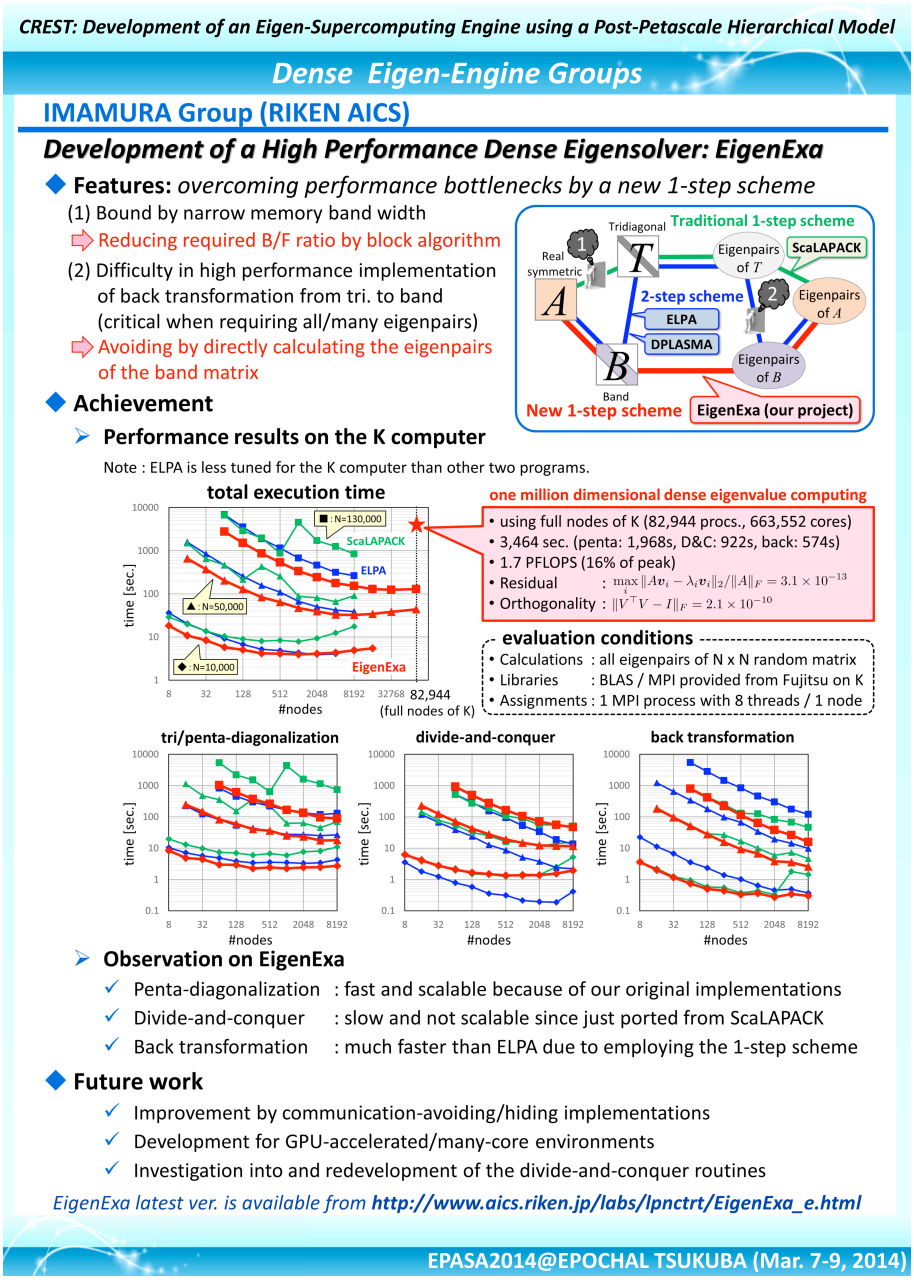


Figure 5. Poster from http://www.aics.riken.jp/labs/lpnctrt/EigenExa_e.html

As you can see the description of "one-million dimensional dense eigenvalue computing", we successfully diagonalized a one-million dimensional random symmetric matrix within one hour by taking account of the full computational nodes of the K computer system. The result shows a favorable properties of the EigenExa library towards the emerging Exa-scale computing era.

2. Theoretical studies and Practices for Communication Avoiding

We have studied basic building blocks of high performance dense eigenvalue solvers. We

have analyzed the parallel performance of our solver to construct a performance model for predicting the performance on a post-peta scale system. In this FY2013-2014, we built a prototype model which estimates the parallel execution time of the most dominant part of our scheme, and we examined its accuracy on K computer (see Figure 6).

We have also studied a communication-avoiding algorithm, called TSQR (or CAQR), for computing a tall-skinny QR factorizations, required in both dense and sparse eigenvalue solvers. We evaluated its performance, particularly the strong scaling, by using K computer. In addition, we pointed out its performance bottleneck by constructing a realistic performance model and are now planning to improve the performance.

Finally, we report our two performance evaluations by using the whole FX10 supercomputer system, Oakleaf-FX, supported by "Large-scale HPC Challenge" Project, Information Technology Center, and the University of Tokyo. In the first one, we measured the performance of EigenExa in various conditions; we changed the size of a target matrix, program parameters such as the shape of process grid and combination of the number of MPI processes and that of the OpenMP threads. In the second one, we compared the performance of TSQR/CAQR with other conventional algorithms such as Householder QR. The results of both evaluations are expected to contribute to further performance tuning of each program.

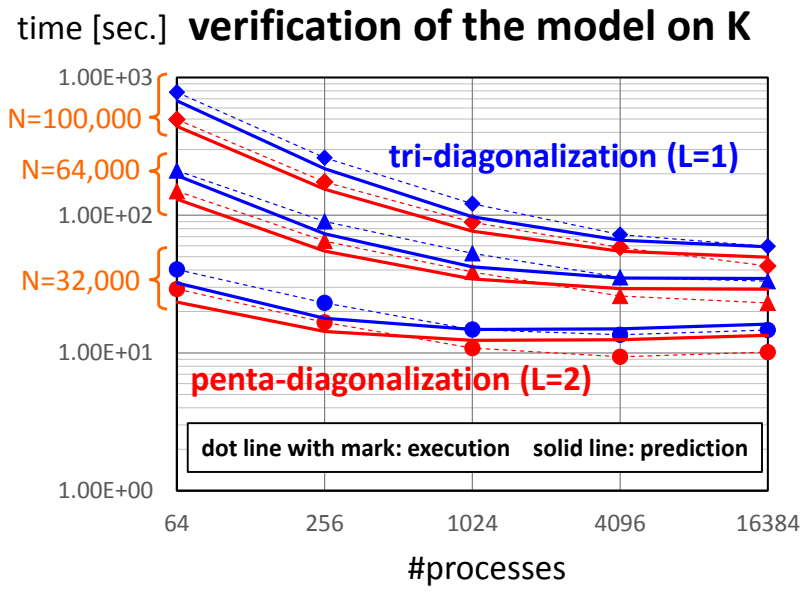


Figure 6. Verification of our performance model on K computer.

3.3 Investigation of the FDTD Related Methods

In order to develop useful mathematical software for K computer, it is significant to investigate

general numerical frameworks not focused on particular simulation codes. FDM (Finite Difference Method) and FEM (Finite Element Method) are well-known numerical discretization and time-integration frameworks for scientific simulation codes, which are based on fixed spatial grid coordination. Other numerical principles to be handled on simulation codes are the particle method and the mesh-less methods. In FY2013-2014, we started the study of the FDTD related issues. This subsection illustrates the current status of our studies.

1. **FDTDM (Finite Difference Time Domain Method)**

   Recent public interests center on the electric power problem, such as an electrical generator, a charge device for an electric vehicle, and side effect of an electromagnetic medical device. Finite Difference Time Domain Method (FDTDM) plays an important role in a numerical simulation of such problems. We recognized that it is one of the key issues to investigate a parallel FDTDM software on K computer while most of the standard FDTDM software is commercial. We mainly conduct 1) numerical analysis of FDTDM, and 2) development of open source software based on FDTDM. Since FY2013-2014, we have investigated the feasibility of FDTDM for numerical simulations.

2. **MTDM (Meshless Time Domain Method)**

   Though FDTDM is a strong numerical scheme for time-dependent electromagnetic simulation, it has a strong restriction on the computational domain. There is a lot of progresses to treat problems in a complex shaped domain, for example, finer meshes or adaptive meshes, etc. Generally, meshless method requires no information about geometrical structure, so an enhancement of FDTDM taking consideration of the meshless framework is an alternative for the numerical simulation in a complex-shaped domain. We study the Meshless Time Domain Method (MTDM) based on the Radial Point Interpolation Method (RPIM). Since FY2013-2014, we have studied the numerical analysis for a 2D simulation and the computational accuracy in terms of 'node distribution' and 'base functions', which are thought as important parameters of MTDM. In addition, we have improved the performance of the MTDM code.

4. Schedule and Future Plan

Our three main projects, KMATHLIB, EigenExa, and FDTD are progressing satisfactorily. They are ongoing projects and there will be some update as follows.

1. **KMATHLIB project**

   In order to promote the KMATHLIB package, we need to support a lot of useful plugged-in OSS. We plan to release the first version of the solver of GEBPs for K computer as a part of

KMATHLIB in FY2014-2015. The generalized eigenvalue solver for dense matrices which comprises the solver for banded matrices will be released in FY2015-2016 or later. Another plan is to develop and release a prototype of the Helmholtz equation solver in FY2014-2015 which is collaborated by the SCALE project.

2. EigenExa project

After the first release of the EigenExa library, several application codes adopt to use EigenExa. We got another important mission to maintain EigenExa continuously. Furthermore, we recognize that it is also significant to improve the performance and scalability. As reported in the last section, we struggled with the communication overhead when the number of processors used is quite large. Towards the post K computer system, HPC researchers, especially who are interested in numerical linear algebra, keep watch on the progress of new technologies such as Communication Avoiding, Communication Hiding, and Synchronous Avoiding. We are going to investigate these in the future EigenExa library.

3. FDTD related method

Our must topics for the FDTD related project are to support a 3D simulation by using MTDM and to analyze computational precision in a practical simulation. In fact, an accurate numerical simulation of side-effects from an MRI device to a human-body has a big impact to life science and medical engineering. We need to promote the FDTD related works to an unexplored field in AICS.

4. Other issues

As we described in the annual report FY2012-2013, "Fault tolerance" or "Resilience" is one of the key words for the peta-scale computing. From the viewpoint of the numerical library, we would like to establish a new algorithmic fault detection mechanism and its framework.

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] Y. Idomura, M. Nakata, S. Yamada, M. Machida, T. Imamura, T. Watanabe, M. Nunami, H. Inoue, S. Tsutsumi, I. Miyoshi, and N. Shida, "Communication overlap techniques for improved strong scaling of gyrokinetic Eulerian code beyond 100k cores on the K-computer", Intl. J. of High Performance Computing Applications (IJHPCA), SAGE publications, Vol. 28, No. 1, pp. 73-86, Feb. 2014. doi: 10.1177/1094342013490973.

(2) Conference Papers

[2] T. Imamura, S. Yamada, and M. Machida, "A High Performance SYMV Kernel on a Fermi-core GPU", High Performance Computing for Computational Science - VECPAR 2012, Lecture Notes in Computer Science, Vol. 7851 (LNCS 7851), pp. 59-71, Springer Verlag, 2013.

[3] S. Yamada, T. Imamura, M. Machida, "Parallel Computing Design for Exact Diagonalization Scheme on Multi-band Hubbard Cluster Models", International Conference on Parallel Computing (ParCo2013), Technische Universiät München, Campus Garching, Munich, Germany, Sep. 10-13, 2013, M. Bader, A. Bode, H.-J. Bungartz, M. Gerndt, G.R. Joubert, F. Peters (eds.): Parallel Computing: Accelerating Computational Science and Engineering (CSE). Advances in Parallel Computing 25, pp. 427-436, IOS Press, 2014.

[4] A. Kuroda, N. Oi, H. Inoue, H. Murai, T. Yamasaki, T. Ohno, T. Imamura, and K. Minami, "Communication Optimization Method on a High-dimensional Mesh/Torus Network for Real Applications --Case Study for the Tofu Network of 'K-computer'--, High Performance Computing Symposium 2014 (HPCS2014), Hitotsubashi-Hall, Tokyo, Jan. 7-8, 2014, IPSJ Symposium Series, Vol. 2014, pp. 97-105, 2013-12-31. (in Japanese)

(3) Invited Talks

[5] T. Imamura, "Roadmap to Eigensolver on a GPU-cluster", GTC Japan 2013, technical session (Research Meeting for GPU Computing organized by GSIC Tokyo Institute of Technology), Tokyo Midtown, Tokyo, Jul. 30, 2013. (in Japanese).

[6] T. Imamura, "Large-scale Eigenvalue solver --from the current status on K computer to upcoming Exa-scale computer ---", Workshop for future HPC (Basic Technologies and Applications), Nagasaki City Library, Nagasaki, Dec. 8-9, 2013. (in Japanese)

[7] T. Imamura, "Communication Avoiding algorithms in numerical linear algebra", 16-th Research Meeting for Matrix Computation Activity Group, JSIAM, the University of Tokyo, Tokyo, Dec. 26, 2013. (in Japanese)

(4) Posters and Presentations

[8] T. Imamura, S. Yamada, and M. Machida, "Eigen-G: GPU-based eigenvalue solver for real-symmetric dense matrices", 10-th International Conference on Parallel Processing and Applied Mathematics (PPAM2014), Polish-Japanese Institute of Information Technology, Warsaw, Poland, Sep. 8-11, 2013. (the paper will be published in Proc., Wyrzykowski, R., Dongarra, J., Karczewski, K., Waśniewski, J. (Eds.), Parallel Processing and Applied Mathematics, Revised Selected Papers, Part I, Lecture Notes in Computer Science, Vol. 8384 (LNCS 8384), Jun. 2014)

[9] T. Imamura, "Automatic Tuning for GPU BLAS kernels", Dagstuhl Seminar, No. 13401 "Automatic Application Tuning for HPC Architectures", Schlöss Dagstuhl, Saarbrucken, Germany, Sep. 29-Oct. 4, 2013. (Oral)

[10] C. Bi, K. Ono, K.-L. Ma, H. Wu, and T. Imamura, "Proper orthogonal decomposition based parallel compression for visualizing big data on the K computer", IEEE Symposium on Large-Scale Data Analysis and Visualization (LDAV 2013), Oct. 13-14, 2013, Atlanta, Georgia, USA, B. Geveci, H. Pfister, and V. Vishwanath (Eds.): Proc. LDAV2013, pp. 121-122, 2013. (Poster)

[11] T. Imamura, S. Yamada, and M Machida, "Strategic study for an O(mega)-core scale parallel eigenvalue solver by using Automatic Tuning technology", 18-th Annual meeting of Japan Society for Computational Engineering and Science, Institute of Industrial Science, the University of Tokyo, Jun. 19-21, 2013, Proc. JSCES, Vol. 18, D-13-5, 2013. (Oral, in Japanese)

[12] N. Sasa, S. Yamada, M. Machida, T. Imamura, and Y. Okuda, "Development and performance evaluation of QPBLAS-GPU", 18-th Annual meeting of Japan Society for Computational Engineering and Science, Institute of Industrial Science, the University of Tokyo, Jun. 19-21, 2013, Proc. JSCES, Vol. 18, D-9-4, 2013. (Oral, in Japanese)

[13] Y. Hirota, and T. Imamura, "Divide and Conquer Method for Generalized Eigenvalue Problems of Banded Matrices", Summer United Workshops on Parallel, Distributed and Cooperative Processing 2013 (SWoPP 2013), Research meeting for Matrix Computation Activity Group, JSIAM, Kitakyushu International Conference Center, Kitakyushu, Jul. 31-Aug. 2, 2013. (Oral, in Japanese)

[14] T. Fukaya, T. Imamura and Y. Yamamoto, "A study on the performance modeling of a dense matrix computation on a massively parallel system", Summer United Workshops on Parallel, Distributed and Cooperative Processing 2013 (SWoPP 2013), Kitakyushu International Conference Center, Kitakyushu, Jul. 31-Aug. 2, 2013, IPSJ SIG Tech. Rep. [High Performance Computing], Vol. 2013-HPC-140, No. 41, pp. 1-8, 2013-07-24. (Oral, in Japanese)

[15] Y. Ohi, T. Tatsuno, and S. Ikuno, "Numerical investigation for stability of electromagnetic field analysis using shape functions based on RPIM", JSIAM 2013 annual meeting, ACROS Fukuoka, Fukuoka, Sep. 9-11, 2013. (Oral, in Japanese)

[16] T. Fukaya, T. Imamura and Y, Yamamoto, "Performance evaluation and estimation of a dense symmetric eigensolver on the K computer", JSIAM annual meeting 2013, ACROS Fukuoka, Fukuoka, Sep. 2013. (Oral, in Japanese)

[17] T. Fukaya, Y. Yamamoto, and T. Imamura, "Performance evaluation of a tall and skinny QR factorization on a large-scale parallel system", 11-th Computational Mathematics Conference, Blanc Art Misasa, Tottori, Nov. 3-4, 2013. (Oral, in Japanese)

[18] Y. Hirota, "On the Divide and Conquer Method for Generalized Eigenvalue Problems and an Extention to the Problems of Banded Matrices", 11th Computational Mathematics Conference, Blanc Art Misasa, Tottori, Nov. 3-4, 2013. (Oral, in Japanese)

[19] Y. Ohi, Y. Fujita, T. Itoh, H. Nakamura, and S. Ikuno, "Speed Up of Shape Function Generation in Meshless Time Domain Method", 23-rd International Toki Conference (ITC-23)

on Large-scale Simulation and Fusion Science, National Institute for Fusion Science, Toki, Japan, Nov. 18-21, 2013. (Poster)

[20] T. Imamura, "Research Activities in AICS towards post Peta-scale Numerical Libraries", 4-th AICS International Symposium, Kobe, Japan, Dec. 2-3, 2013. (Oral)

[21] Y. Ohi, T. Itoh, and S. Ikuno, "Speedup for Generation of Shape Function in Meshless Time Domain Method – Application for a circular sector domain having constant curvature", Nonlinearity/ Visualization-Section Meeting in Workshop on developments of simulation methods for plasma-wall interaction 2013, National Institute for Fusion Science, Toki, Dec. 9-10, 2013. (Oral, in Japanese)

[22] T. Fukaya, Y. Yamamoto and T. Imamura, "A TSQR algorithm based on the Gram-Schmidt orthogonalization and its performance evaluation", 16-th Research Meeting for Matrix Computation Activity Group, JSIAM, the University of Tokyo, Tokyo, Dec. 26, 2013. (Oral, in Japanese)

[23] K. Okada, Y. Okamoto, and T. Imamura, "Optimization of the format of input matrix for CRS-based Matrix-Vector multiplication on a multi-GPU environment", High Performance Computing Symposium 2014 (HPCS2014), Hitotsubashi-Hall, Tokyo, Jan. 7-8, 2014, IPSJ Symposium Series, Vol. 2014, pp. 28, 2013-12-31. (Poster, in Japanese)

[24] K. Shirosawa, T. Imamura, and Y. Okamoto, "Thread parallelization of a successive band reduction method for real-symmetric matrices on a multi-core CPU", High Performance Computing Symposium 2014 (HPCS2014), Hitotsubashi-Hall, Tokyo, Jan. 7-8, 2014, IPSJ Symposium Series, Vol. 2014, pp. 29, 2013-12-31. (Poster, in Japanese)

[25] X. Lin, T. Imamura, and Y. Okamoto, "Performance tuning strategy for GEMV kernels by using d-Spline function", High Performance Computing Symposium 2014 (HPCS2014), Hitotsubashi-Hall, Tokyo, Jan. 7-8, 2014, IPSJ Symposium Series, Vol. 2014, pp. 30, 2013-12-31 (Poster, in Japanese)

[26] T. Imamura, and Y. Hirota, "Communication Avoiding-hiding and Auto-tuning for Extreme-scale Eigensolver", SIAM Conference on Parallel Processing for Scientific Computing (PP14), Portland, OR, USA, Feb. 20, 2014. (Oral)

[27] T. Fukaya, and Y. Yamamoto, "Auto-tuning Tall and Skinny QR Factorization", SIAM Conference on Parallel Processing for Scientific Computing (PP14), Portland, OR, USA, Feb. 20, 2014. (Oral)

[28] R. Tamura, T. Imamura, and Y. Nakatani, "Study for TSQR algorithm by Fully Offload model onto a GPU", 143-th SIGHPC IPSJ (HPC143), Ae-no-Kaze, Wakura-Onsen, Mar. 3-4, 2014, IPSJ SIG Tech. Rep. [High Performance Computing], Vol. 2014-HPC-143, No. 21, pp. 1-7, 2014-02-24. (Oral)

[29] T. Sakurai, S.-L. Zhang, T. Imamura, Y. Yamamoto, Y. Kuramashi, and T. Hoshi, CREST project, "Development of an Eigen-Supercomputing Engine using a Post-Petascale Hierarchical

Model", International Workshop on Eigenvalue Problems: Algorithms; Software and Applications, in Petascale Computing (EPASA 2014), Epochal Tsukuba, Tsukuba, Japan, Mar. 7-9, 2014. (Oral)

[30] T. Sakurai, S.-L. Zhang, T. Imamura, Y. Yamamoto, Y. Kuramashi, and T. Hoshi, CREST project, "Development of an Eigen-Supercomputing Engine using a Post-Petascale Hierarchical Model", EPASA2014, Tsukuba, Japan, Mar. 7-9, 2014. (Poster)

[31] T. Imamura, and Y. Yamamoto, "CREST: Dense Eigen-Engine Groups", EPASA2014, Tsukuba, Japan, Mar. 7-9, 2014. (Poster)

[32] Y. Hirota, and T. Imamura, "Divide and Conquer Method for Computing Generalized Eigenvalues of Banded Matrices", EPASA2014, Tsukuba, Japan, Mar. 7-9, 2014. (Poster)

[33] T. Fukaya, Y. Yamamoto, and T. Imamura, "An overview of parallel algorithms for tall-skinny QR factorizations", EPASA2014, Tsukuba, Japan, Mar. 7-9, 2014. (Poster)

[34] Y. Yanagisawa, Y. Nakatsukasa, and T. Fukaya, "Cholesky-QR and Householder-QR factorizations in nonstandard inner product spaces", EPASA2014, Tsukuba, Japan, Mar. 7-9, 2014. (Poster)

[35] T. Imamura, "Development of a high performance eigenvalue solver on third generation NVIDIA GPU's", Material Design through Computics: Complex Correlation and Non-equilibrium Dynamics, Scientific Research on Innovative Areas, a MEXT Grant-in-Aid Project FY2010-2014, 2-nd Research Meeting in FY2013-2014, the University of Tokyo, Tokyo, Mar. 11, 2014. (Oral, in Japanese)

[36] T. Imamura, "Automatic-tuning for CUDA-BLAS kernels by Multi-stage d-Spline Pruning Strategy", 2014 Conference on Advanced Topics and Auto Tuning in High Performance Scientific Computing, (2014 ATAT in HPSC), National Taiwan University, Taipei, Taiwan, Mar. 14-15, 2014. (Oral)

[37] T. Fukaya, "A Communication-Avoiding Algorithm for the Gram-Schmidt Orthogonalization", 2014 Conference on Advanced Topics and Auto Tuning in High Performance Scientific Computing, (2014 ATAT in HPSC), National Taiwan University, Taipei, Taiwan, Mar. 14-15, 2014. (Oral)

[38] Y. Hirota, and T. Imamura, "On Numerical Solution Methods for the Secular Equation Appearing in Divide and Conquer Method for Generalized Eigenvalue Problems", 10th Joint Symposium of JSIAM Activity Groups, Kyoto University, Kyoto, Mar. 19-20, 2014. (Oral, in Japanese)

(5) Patents and Deliverables

[39] EigenExa, http://www.aics.riken.jp/labs/lpnctrt/EigenExa_e.html

HPC Usability Research Team

1. Team Members

Toshiyuki Maeda (Team Leader)

Masatomo Hashimoto (Research Scientist)

Tatsuya Abe (Research Scientist)

Petr Bryzgalov (Research Scientist)

Itaru Kitayama (Technical Staff I)

Yves Caniou (Visiting Scientist, University of Tokyo)

Yoshiki Nishikawa (Visiting Scientist, University of Tokyo)

Sachiko Kikumoto (Assistant)

2. Research Activities

The mission of the HPC Usability Research Team is to research and develop a framework and its theories/technologies for liberating large-scale HPC (high-performance computing) to end-users and developers. In order to achieve the goal, we conduct research in the following three fields:

1. **Computing portal**

   In a conventional HPC usage scenario, users live in a closed world. That is, users have to play roles of software developers, service providers, data suppliers, and end users. Therefore, a very limited number of skilled HPC elites can enjoy the power of HPC, while the general public sometimes gives a suspicious look to the benefit of HPC. In order to address the problem, we are designing and implementing a computing portal framework that lowers the threshold for using, providing, and aggregating computing/data services on HPC systems, and liberates the power of HPC to the public.

2. **Virtualization**

   Virtualization is a technology for realizing virtual computers on real (physical) computers. One big problem of the above mentioned computer portal that can be used by wide range of users simultaneously is how to ensure safety, security, and fairness among multiple users and computing/data service providers. In order to solve the problem, we plan to utilize the virtualization technology because virtual computers are isolated from each other, thus it is easier to ensure safety and security. Moreover, resource allocation can be more flexible than the conventional job scheduling because resource can be allocated in a find-grained and dynamic way. We also study lightweight virtualization techniques for realizing virtual large-scale HPC for test, debug, and verification of computing/data services.

3. Program analysis/verification

Program analysis/verification is a technology that tries to prove certain properties of programs by analyzing them. By utilizing software verification techniques, we can prove that a program does not contain a certain kind of bug. For example, the byte-code verification of Java VM ensures memory safety of programs. That is, programs that pass the verification never perform illegal memory operations at runtime. Another big problem of the above mentioned computing portal framework is that one computing service can be consists of multiple computing services that are provided by different providers. Therefore, if a bug or malicious attack code is contained in one of the computing services, it may affect the whole computing service (or the entire portal system). In order to address the problem, we plan to research and develop software verification technologies for large-scale parallel programs. In addition, we also plan to research and develop a performance analysis and tuning technology based on source code modification history.

3. Research Results and Achievements

3.1. Design and Implementation of a Computing Portal Framework for HPC

Based on the prototype design and implementation of a computing portal framework in FY2012, we actually developed a prototype user-interface for the computing portal framework. More specifically, we implemented a web interface that runs on users' web browsers and directly communicates with the backend system of the computing portal under the protocol (also designed in FY2012). With the web interface, software developers can easily publish their applications installed in HPC systems. For example, developers can specify the paths to the executables of their applications, parameters of their applications, and so on, via the web interface. In addition, developers can manage user accounts that are allowed to execute their applications. With the same web interface, users are also able to launch jobs. For example, users can select an application published in the computing portal, make an application to developers for using it, launch jobs by executing the application with arbitrary parameters, and manage the launched/exited jobs.

One feature of our computing portal framework is that the communication protocol between the framework and its clients is based on the popular web-based application frameworks (e.g., WebSockets, JSON, etc.). Therefore, developers can develop their own custom interfaces for their applications if the web interface of our framework does not satisfy their requirements. Another distinguishing feature of our framework is that users can use portable devices (e.g., smartphones, mobile tablets, and so on) because our web interface is carefully designed so that it can be viewed and accessed with any screen size.

One big limitation of our current computing portal framework is that security mechanisms are still not introduced. That is, (maybe malicious) users and/or applications can easily access the other users/applications data. This problem has been already recognized in FY2012, but we have not addressed the problem directly in our prototype framework. Instead, in FY2013, we studied so-called container (or sandbox) mechanisms, that enable users to isolate their computing environments from other users. As a first step, we investigated a lightweight container system called Docker (https://www.docker.io/), and implemented a utility tool which is able to give every user an isolated computing environment in the form of a container of Docker.

In FY2014, we will continue to develop our computing portal framework. Especially, we plan to integrate some kind of security mechanism (e.g., Docker, if possible) to our framework. We also plan to integrate our framework to the real K computer, but we recognize that it is not so easy from the viewpoint of the operation policy of the K computer.

3.2. Virtualization Techniques

1. **Lightweight virtualization for testing/debugging parallel programs**

   Writing a program for massively parallel HPC environments (e.g., K computer) is a hard task. This is mainly because parallel programs inherently have non-determinacy, thus, it is sometimes extremely difficult to debug a bug in parallel programs, because the bug may not be easily reproducible. In addition to the hard-to-debug problem, there is also a performance problem in writing massively parallel programs. It is not uncommon that, even if a program scales on a PC cluster system whose size is small-to-moderate, the performance of the program severely degrades on massively parallel HPC systems. This is because communication costs between computing nodes may largely vary and sometimes incurs unacceptable heavy overheads.

   In order to address the problem, we have been developing a lightweight network virtualization system for testing/debugging programs for massively parallel programs without actually using real massively parallel HPC environments. With our system, users can run several hundreds of virtual computing nodes on a single physical computing node.

   One key idea of our lightweight virtualization system is to utilize the library-hooking approach, that is, intercept function calls for network related operations from user programs, and modify parameters and/or return values of the function calls in order to "trick" the user programs as if they are executed in isolated virtual computing nodes, even

though they run on a single computing node. One benefit of the library-hooking approach is that it introduces little overheads to program execution (compared to other virtualization techniques, e.g., CPU level virtualization, OS level virtualization, and so on) because it can be achieved by user-level operations only and requires no interaction with OS.

Another key idea of our lightweight virtualization system is reduction of the costs of network routing management by statically distributing routing information as much as possible. The routing information is necessary to correctly route network packets from one virtual node to another where they may reside in different physical computing node. Therefore, if the routing information is maintained by one single physical node, all the physical nodes have to communicate with the manager node each time they need to route packets from one virtual node to another, thus the node results in a performance bottleneck.

In order to address the problem, our lightweight virtualization system statically distributes the routing information as much as possible before executing user programs on virtual computing nodes. In ordinary HPC environments, the network topology of each job execution is fixed during the job execution. Therefore, our static distribution of the routing information should work in most cases. Even if some jobs require dynamic node allocation, our system tries to minimize the cost of updating the routing information by carefully allocating virtual network port. More concretely, we first divide the range of the available network ports into disjoint ranges, and allocate the divided range to each physical computing node.

Based on the above approaches, in FY2013, we have implemented a prototype of our lightweight virtualization system. Although there still remain bugs, it successfully runs on conventional PC clusters and Fujitsu's FX10. More specifically, several MPI applications (including some of the NAS parallel benchmarks (NPB)) ran on our prototype virtualization system. In addition, we also ran Scalasca (a network performance profiling tool) on our system.

In FY2014, we will continue the development of our system and plan to study an approach of tricking performance profiling tools so that they feel as if they run on real computing nodes and emit profiling data which represents characteristics of real massively-parallel computing environments.

2. CPU emulators for SPARC 64 VIIIfx

One big problem of the current K computer from the viewpoint of usability is that it adopted SPARC architecture (more precisely, SPARC 64 VIIIfx architecture), which is rarely used in ordinary PCs, servers, and HPC (they are almost dominated by Intel architectures). Therefore, in order to utilize the K computer, ordinary users have to prepare source code of applications that they want to run, cross-compile the source code on the front-end node of the K computer because binary executables for Intel architecture do not run on SPARC architecture directly. To make things worse, cross-compilation of applications sometimes produce malfunctioning executables partly because the applications do not consider CPU architectures but Intel architecture. Therefore, users have to test the cross-compiled executables on the K computer whether they work expectedly or not.

In order to address the problem, we are studying on CPU emulators. A CPU emulator is a program which emulates the effects of instructions of a CPU architecture. More specifically, we are working on two kinds of CPU emulators. One is a CPU emulator which emulates SPARC 64 VIIIfx on Intel architecture, and another is a CPU emulator which emulates Intel architecture on SPARC 64 VIIIfx. With the former SPARC 64 VIIIfx on Intel emulator, users are able to test the cross-compiled executables for the K computer on their own development environments (PC, clusters, and so on). With the latter Intel on SPARC 64 VIIIfx emulator, users are able to run their binary executables for Intel architecture on the K computer without cross-compiling their source code.

More concretely, we are developing the two emulators by extending the existing CPU emulator QEMU. For the SPARC 64 VIIIfx on Intel emulator, we extended QEMU to support the features specific to the SPARC 64 VIIIfx architecture (e.g., extended general purpose/floating-pointer registers, SIMD extension, and so on). For the Intel on SPARC 64 VIIIfx, we fixed bugs of QEMU that prevents normal operations of QEMU on the K computer.

In FY2013, we continued development of the SPARC 64 VIIIfx on Intel emulator from FY2012, but we could not complete the development (there still remain several severe bugs that prevent many applications from working). On the other hand, the prototype implementation of the Intel on SPARC VIIIfx emulator has been completed and several applications successfully run on the emulator. However, its performance is not satisfactory because its execution time is 10 to 20 times slower.

In FY2014, we will continue the development of the two CPU emulators. For the SPARC 64

VIIIfx on Intel emulator, we aim to implement a more stable system which is usable for practical testing of applications that should be executed on the K computer. For the Intel on SPARC 64 VIIIfx emulator, we will improve its execution performance.

3.3. Program verification and analysis

1. Memory Consistency Model-Aware Program Verification

A memory consistency model is a formal model which specifies the behavior of the shared memory which is simultaneously accessed by multiple threads and/or processes. The recent multicore CPU architectures and shared memory multithread/distributed programming languages (e.g., Java, C++, UPC, Coarray Fortran, and so on) adopt *relaxed* memory consistency models. Under the relaxed memory consistency models, the shared memory sometimes behaves very differently from non-relaxed, sequential memory consistency models. For example, under some relaxed memory consistency models, the effects of the memory operations (e.g., A→B) performed sequentially by one thread may be observed in a different order (e.g., B→A) by the other threads. In addition, the threads may not agree on the observation orders of the effects of the memory operations (e.g., one thread observes A→B, while the other observes B→A, and so on). The reason why the recent CPUs and shared memory languages adopt relaxed memory consistency models is that a large number of threads and/or nodes share a single address memory space, thus enforcing non-relaxed, sequential memory consistency incurs huge synchronization overheads among the threads/nodes.

From the viewpoint of program verification, there are two problems in handling relaxed memory consistency models. First problem is that the conventional program verification approaches do not consider relaxed memory consistency models. Thus, they cannot be applied to relaxed memory consistency models because they may yield false results. Second problem is that there exist various kinds of relaxed memory consistency models and each CPU architecture/each programming language adopts different memory consistency models from each other. Therefore, it is tedious to define and implement a program verification approach for each CPU and programming languages of relaxed memory consistency models.

To address the problem, in FY2013, we studied three approaches. First approach is to define a new formal system which is able to represent various relaxed memory consistency models. More specifically, we define a very relaxed memory consistency model as a base model. On top of the base model, we defined various memory consistency models as

additional axioms. With our formal system, we are able to define a broad range of memory consistency models from CPUs to shared-memory programming languages (e.g, Intel64, Itanium, UPC, Coarray Fortran, and so on), in the single formal system. With our formal system, we were able to proof the correctness of Dekker's mutual exclusion algorithm under the memory consistency model of Itanium.

Second approach is to design and implement a model checker which supports various relaxed memory consistency models based on the formal model of the first approach. More specifically, we define a non-deterministic state transition system with execution traces where each execution trace represents a possible permutation of instruction executions. Roughly speaking, given a target program, our model checker explores all the reachable states in the non-deterministic transition system of the target problem for all the possible execution traces (that is, permutations of instructions). In our model checker, memory consistency models can be defined as constraint rules on execution traces. For example, the sequential consistency model can be defined as a constraint which allows no permutation on the execution traces. With our model checker, we were able to verify the small examples programs of the specification manuals of the memory consistency models of Itanium and UPC. In addition, we were also able to formally discuss comparison of the two memory consistency models (Itanium and UPC).

Third approach is to define a new Hoare-style logic for a shared-memory parallel process calculus under a relaxed memory consistency model. More specifically, we define an operational semantics for the process calculus. Then define a sound (and relatively-complete) logic to the semantics. There are two key ideas in our Hoare-style logic. First idea is that a program is translated into a dependence graph among instructions in the program, and the operational semantics and the logic are defined in terms of the dependence graph. One advantage of handling dependence graphs is that while loops, branch statements, and parallel composition of processes can be handled in a uniform way. In addition, another advantage is that multiple memory consistency models can be handled by adopting different translation approaches for each memory consistency model. Second idea is that we introduce auxiliary variables in the operational semantics that temporarily buffer the effects of memory operations. Based on our Hoare-style logic, we also implemented a prototype semi-automatic theorem prover.

2. Evidence-Based Performance Tuning

In order to fully utilize the power of HPC systems, it is necessary to optimize and tune the performance of applications. However, performance tuning is a troublesome task because,

even if performance bottlenecks/hotspots can be detected by performance profiling, it is not apparent how to rewrite programs to remove the bottlenecks/hotspots. In addition, generally speaking, modifying correctly working programs is reluctant from the viewpoint of developers. Thus, performance tuning requires experienced craftsmanship, and relies on intuition and experience.

In order to address the problem, we are working on an idea of evidence-based performance tuning. More specifically, we store the results of performance profiling in a database where the results are associated with source code modification history. With the database, developers are able to know, for example, what kinds of optimization were applied in the past, what kinds of optimization are effective for improving a certain performance profiling parameter, and so on. In FY2013, we conducted a preliminary experiment to implement the database and obtained promising results. However, because the experiment was still very preliminary with very little number of application programs, we do not have full confidence, so far. In FY2014, we plan to conduct the more realistic experiment with larger number of applications with more realistic source code modification histories.

4. Schedule and Future Plan

In FY 2014, we will improve the prototype implementation of our computing portal. As mentioned above, the current implementation does not have rigid security mechanism. In order to address the security problem, we will modify and/or extend the current APIs/protocols of our computing portal and apply them to the implementation. In addition, we will also consider integrating a security sandbox system (e.g., Docker) to our implementation. Besides the security problem, we also plan to integrate our framework to the real K computer, if our security and political policies allow.

Regarding the virtualization technologies, we will continue to implement the lightweight network virtualization framework for testing/debugging parallel programs. Especially, we will design and implement a mechanism which tricks performance profiling tools so that they feel as if they run on real computing nodes and emit profiling data which represents characteristics of real massively parallel computing environments. In addition, we will also continue to implement the SPARC 64 VIIIfx on Intel emulator and Intel on SPARC 64 VIIIfx emulators.

Regarding the program verification and analysis, we will conduct more experiments with our three approaches for program verification under relaxed memory consistency models to evaluate their effectiveness and practicality. In addition, we will also consider designing and

implementing a more simple and concise logic/model based on the experiences of the three approaches. Regarding the evidence-based performance tuning, we plan to conduct the more realistic experiment with larger number of applications with more realistic source code modification histories with the prototype implementation developed in FY2013.

In addition to the above mentioned individual research topics, we plan to start integrating the research results of the virtualization technologies and the software verification into the computing portal somewhere from the second half of FY 2014 to the first half of FY 2015.

5. Publication, Presentation and Deliverables

(1) Conference Papers

[1] Abe, T. and Maeda, T., "Model Checking Stencil Computations Written in a Partitioned Global Address Space Language", In Proceedings of the 18th International Workshop on High-Level Parallel Programming Models and Supportive Environments (HIPS 2013).

[2] Abe, T. and Maeda, T., "Model Checking with User-Definable Memory Consistency Models", In Proceedings of the 6th Conference on Partitioned Global Address Space Programming Models (PGAS 2013), Short paper, online.

[3] Abe, T. and Maeda, T., "A General Model Checking Framework for Various Memory Consistency Models", In Proceedings of the 19th International Workshop on High-Level Parallel Programming Models and Supportive Environments (HIPS 2014). To appear.

(2) Presentations

[4] Kitayama, I., "A User's Experience with FEFS", In Japan LUG (Lustre User Group) 2013.

[5] Maeda, T., "Brief Introduction of HPC Usability Research Team", In the 4th AICS International Symposium, 2013.

(3) Software

[6] K-scope with SSHConnect (joint work with Software Development team of AICS):
URL: http://www.kcomputer.jp/ungi/soft/kscope/

[7] Python binding of EigenExa (joint work with Dr. Shimazaki of Computational Molecular Science Research Team of AICS. Partially feedbacked to the original developers of Large-scale Parallel Numerical Computing Technology Research Team)

[8] DockerIaaStool: Tools for creating a simple Infrastructure-as-a-Service system with Docker
URL: https://github.com/pyotr777/dockerIaaSTools

[9] QEMU on the K computer: CPU emulator for executing Intel binary executables on the K computer (implemented by extending the original QEMU emulator. In preparation for publication.)

[10] ABySS on the K computer: Parallel, paired-end sequence assembler (implemented by modifying the original ABySS so that it scales on the K computer. In preparation for publication.)

Field Theory Research Team

1. Team members

Yoshinobu Kuramashi (Team Leader)

Yoshifumi Nakamura (Research Scientist)

Hiroya Suno (Research Scientist, Joint Position with the Nishina Center for Accelerator-based Research)

Xia-Yong Jin (Postdoctoral Researcher)

Jarno Markku Olavi Rantaharju (Postdoctoral Researcher)

Yuya Shimizu (Postdoctoral Researcher)

Ken-Ichi Ishikawa (Visiting Scientist)

Takeshi Yamazaki (Visiting Scientist)

Shinji Takeda (Visiting Scientist)

2. Research Activities

Our research field is physics of elementary particles and nuclei, which tries to answer questions in history of mankind: What is the smallest component of matter and what is the most fundamental interactions? This research subject is related to the early universe and the nucleosynthesis through Big Bang cosmology. Another important aspect is quantum properties, which play an essential role in the world of elementary particles and nuclei as well as in the material physics at the atomic or molecular level. We investigate nonperturbative properties of elementary particles and nuclei through numerical simulations with the use of lattice QCD (Quantum ChromoDynamics). The research is performed in collaboration with applied mathematicians, who are experts in developing and improving algorithms, and computer scientists responsible for research and development of software and hardware systems.

Lattice QCD is one of the most advanced case in quantum sciences: Interactions between quarks, which are elementary particles known to date, are described by QCD formulated with the quantum field theory. We currently focus on two research subjects: (1) QCD at finite temperature and finite density. We try to understand the early universe and the inside of neutron star by investigating the phase structure and the equation of state. (2) First principle calculation of nuclei based on QCD. Nuclei are bound states of protons and neutrons which consist of three quarks. We investigate the hierarchical structure of nuclei through the direct construction of nuclei in terms of quarks.

Successful numerical simulations heavily depend on an increase of computer performance by

improving algorithms and computational techniques. However, we now face a tough problem that the trend of computer architecture becomes large-scale hierarchical parallel structures consisting of tens of thousands of nodes which individually have increasing number of cores in CPU and arithmetic accelerators with even higher degree of parallelism: We need to develop a new type of algorithms and computational techniques, which should be different from the conventional ones, to achieve better computer performance. For optimized use of K computer our research team aims at (1) developing a Monte Carlo algorithm to simulate physical system with negative weight effectively and (2) improving iterative methods to solve large system of linear equations. These technical development and improvement are carried out in the research of physics of elementary particles and nuclei based on lattice QCD.

3. Research Results and Achievements

3.1. QCD at finite temperature and finite density

Establishing the QCD phase diagram spanned by the temperature T and the quark chemical potentialμin a quantitative way is an important task of lattice QCD. The Monte Carlo simulation technique, which has been successfully applied to the finite temperature phase transition studies in lattice QCD, cannot be directly applied to the finite density case due to the complexity of the quark determinant for finiteμ. Recently we investigated the phase of the quark determinant with finite chemical potential in lattice QCD using an analytic method: Employing the winding expansion and the hopping parameter expansion to the logarithm of the determinant, we have shown that the absolute value of the phase has an upper bound that grows with the spatial volume but decreases exponentially with an increase in the temporal extent of the lattice. Based on this analysis we carried out a finite size scaling study for 4 flavor QCD using the O(a) improved Wilson quark action and the Iwasaki gauge action. This was the first application of the finite size scaling study to the finite density QCD. After the study of 4 flavor QCD we have moved to 3 flavor case. The main target is to trace the critical end line in the parameter space of temperature, chemical potential and hopping parameter (quark mass). We employ two strategies to determine the critical end point in simulation with fixed chemical potential. One is to identify at which temperature the Binder cumulant/Kurtosis measured at the transition point on two different spatial volumes intersects. This method is based on the property of opposite spatial volume dependence of the Binder cumulant/Kurtosis at the transition point between the first order phase transition side and the crossover one. The other is to locate the critical temperature where a gap of transition point for two observables potentially allowed in the crossover side vanishes. Physical observables are calculated with the phase reweighting method. We evaluate the phase of determinant exactly by developing an efficient numerical technique with the use of a dimensional reduction of temporal direction.

3.2. Nuclei in lattice QCD

In 2010 we succeeded in a direct construction of the ^{4}He and ^{3}He nuclei from quarks and gluons in lattice QCD for the first time. Calculations were carried out at a rather heavy degenerate up and down quark mass corresponding to m_π=0.8 GeV in quenched QCD to control statistical errors in the Monte Carlo evaluation of the helium Green's functions. As a next step we investigated the dynamical quark effects on the binding energies of the helium nuclei, the deuteron and the dineutron. We performed a 2+1 flavor lattice QCD simulation with the degenerate up and down quark mass corresponding to m_π=0.51 GeV. To distinguish a bound state from an attractive scattering state, we investigate the spatial volume dependence of the energy difference between the ground state and the free multi-nucleon state by changing the spatial extent of the lattice from 2.9 fm to 5.8 fm. We observed that the measured ground states for all the channels are bound. This result raises an issue concerning the quark mass dependence. At the physical quark mass, there is no bound state in the dineutron channel. So we expect that the bound state in the dineutron channel observed in our simulation at m_π=0.51 GeV have to disappear at some quark mass toward the physical value. We are now investigating the quark mass dependence performing a simulation at m_π=0.30 GeV.

3.3. Development of algorithms and computational techniques

3.3.1. Iterative method to solve large system of linear equations

We consider to solve the linear systems with multiple right-hand sides expressed as AX=B, where A is an N×N matrix and X, B are N×L matrices with L the number of multiple right-hand side vectors. Various fields in computational sciences face this type of problem. In lattice QCD simulations, for example, one of the most time consuming part is to solve the Wilson-Dirac equation with the multiple right-hand sides, where A is an N×N complex sparse non-Hermitian matrix and X, B are N×L complex matrices with N the number of four dimensional space-time sites multiplied by 12. We aim at reducing the computational cost with the block Krylov subspace method which makes convergence faster than the non-blocked method with the aid of better search vectors generated from wider Krylov subspace enlarged by the number of multiple right-hand side vectors. We improve the block BiCGSTAB algorithm with the QR decomposition. After an optimization of the matrix-vector multiplication on K computer, the sustained performance for the block solver has reached nearly 35% of theoretical peak performance for a 12^3×24 lattice on 16 nodes. As a next step we have applied the block BiCGSTAB with the QR decomposition to a real problem in lattice QCD. We employ a set of configurations generated at almost the physical point (κ_{ud},κ_s) = (0.126117,0.124790) on 96^4 in 2+1 flavor lattice QCD using the nonperturbatively O(a) improved Wilson quark action with c_{SW}=1.11 and the Iwasaki gauge action at β=1.82. Stout smearing procedure is employed with the parameters N_{stout}=6 and α=0.1. Our numerical test is performed on 2048 nodes on the K

computer so that each node has a $12^3 \times 24$ lattice. Table I shows the L dependence of the computational cost to solve the Wilson-Dirac equation. We find that both the number of inner matrix-vector multiplications and the computational time divided by L decrease by about 15% as L increases from 1 to 12.

We have applied the optimization technique acquired in lattice QCD to RSDFT (Real Space Density Functional Theory) which is widely used to calculate ground state energies of the quantum many body states in the condensed matter physics and the nuclear physics. The sustained performance for the matrix-vector multiplication part in the RSDFT code is successfully increased from 3.0% to 8.3%. This work is done in collaboration with Sakurai group at University of Tsukuba who are developing a massively parallel eigenvalue analysis engine for post-petascale machines with a hierarchical parallel structure under a research area of the CREST program "Development of System Software Technologies for post-Peta Scale High Performance Computing".

Table 1: L dependence of the number of inner matrix-vector multiplications (IMVMs) and execution time to solve the Wilson-Dirac equation.

L	#IMVM	time [s]	time/L [s]
1	915.3	65.2	65.2
2	913.0	128.4	64.2
3	876.8	193.8	64.6
4	869.7	235.6	58.9
6	856.5	349.3	58.2
12	770.0	669.0	55.8

3.3.2. Algorithm to simulate physical system with negative weight in path-integral formalism

The Schwinger model, two-dimensional QED, has been used as a theoretical test bed for QCD. It has many QCD-like properties: confinement for fermions, chiral symmetry breaking due to the $U_A(1)$ anomaly, etc. The lattice regularized version of the Schwinger model is also favorable for the development of numerical techniques to tackle lattice QCD. The hybrid Monte Carlo algorithm (HMC) is the most successful method to implement dynamical fermions so far. However, it loses validity when the determinant of the lattice-regularized Dirac matrix can be negative. Such a difficulty has been preventing us from studying the phase structure of the

one-flavor lattice Schwinger model in the Wilson fermion formulation with the HMC algorithm. We apply the Grassmann tensor renormalization group to the lattice Schwinger model with one-flavor of the Wilson fermion. We demonstrate that the GTRG works well even at the critical hopping parameter where the negative sign from the fermion determinant may arise, and determines the phase structure of the one-flavor lattice Schwinger model. This is the first application of the GTRG to lattice gauge theory including fermions. Since it has been shown that the GTRG has a strong advantage that it does not suffer from the sign problem caused by the fermion determinant, next step may be an application of the GTRG to the physical system with the so-calledθterm where the action is a complex number. A numerical analysis of the lattice Schwinger model with theθterm is under way.

4. Schedule and Future Plan

4.1. QCD at finite temperature and finite density

After finishing the investigation of 3 flavor QCD, we plan to explore the analysis of the phase structure in 2+1 flavor QCD with the finite size scaling study. We will focus on the determination of the critical surface in the parameter space of temperature, chemical potential and hopping parameters (quark masses).

4.2. Nuclei in lattice QCD

Our preliminary results at m_π=0.30 GeV in 2+1 flavor QCD show that the dineutron channel seems still bound. We plan to make a large scale simulation at or around the physical quark mass.

4.3. Development of algorithms and computational techniques

4.3.1. Iterative method to solve large system of linear equations

As mentioned at the end of Sec. 3.3.1, Sakurai group at University of Tsukuba are developing software packages for massively parallel eigenvalue computation, one of which is z-Pares (short for Complex Moment-based Parallel Eigen-Solvers). In collaboration with his group we try to apply the z-Pares to an eigenvalue analysis of the Wilson-Dirac operator on a 96^4 lattice in 2+1 flavor lattice QCD on K computer.

4.3.2. Algorithm to simulate physical system with negative weight in path-integral formalism

We are now applying the GTRG method to the Schwinger model with theθterm. Once the GTRG method is proved to be efficient even for the complex action, next step is an extension to the SU(3) gauge theory.

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] X-Y. Jin, Y. Kuramashi, Y. Nakamura, S. Takeda, and A. Ukawa, "Finite size scaling study of N_f=4 finite density QCD on the lattice", Physical Review D88 (2013) 094508.

[2] Yuya Shimizu and Yoshinobu Kuramashi, "Grassmann Tensor Renormalization Group Approach to One-Flavor Lattice Schwinger Model", arXiv:1403.0642 [hep-lat].

[3] H. Suno, E. Hiyama, and M. Kamimura, "Theoretical Study of Triatomic Systems Involving Helium Atoms", Few-Body Systems 54 (2013) 1557.

[4] H. Suno, "A Theoretical Study of Pure and Mixed Spin-Polarized Tritium and Helium Triatomic Systems Using Hyperspherical Coordinates", Few-Body Systems 55 (2014) 229.

(2) Conference Papers

[5] S. Takeda, X-Y. Jin, Y. Kuramashi, Y. Nakamura, and A. Ukawa, "Finite size scaling for 3 and 4-flavor QCD with finite chemical potential", Proceedings of Science (Lattice 2013) 203.

[6] Xiao-Yong Jin, Yoshinobu Kuramashi, Yoshifumi Nakamura, Shinji Takeda, and Akira Ukawa, "Zeros of QCD partition function from finite density lattices", Proceedings of Science (Lattice 2013) 204.

[7] T. Yamazaki, K.-I. Ishikawa, Y. Kuramashi, and A. Ukawa, "Multi-nucleon bound states in N_f=2+1 lattice QCD", Proceedings of Science (Lattice 2013) 230.

[8] R. Horsley, J. Najjar, Y. Nakamura, H. Perlt, D. Pleiter, P.E.L. Rakow, G. Schierholz, A. Schiller, H. Stüben, and J.M. Zanotti, "SU(3) flavour symmetry breaking and charmed states", Proceedings of Science (Lattice 2013) 249.

[9] A.N. Cooke, R. Horsley, Y. Nakamura, D. Pleiter, P.E.L. Rakow, P. Shanahan, G. Schierholz, H. Stüben, and J.M. Zanotti, "SU(3) flavour breaking and baryon structure", Proceedings of Science (Lattice 2013) 278.

[10] R. Horsley, Y. Nakamura, D. Pleiter, P.E.L. Rakow, G. Schierholz, H. Stüben, R.D. Young, and J.M. Zanotti, "Electromagnetic splitting of quark and pseudoscalar meson masses from dynamical QCD + QED", Proceedings of Science (Lattice 2013) 499.

[11] Jarno Rantaharju, "The Gradient Flow Coupling in Minimal Walking Technicolor", Proceedings of Science (Lattice 2013) 084.

(3) Invited Talks

[12] Y. Kuramashi, "Lattice QCD – From Quarks to Nuclei –", University of Tsukuba and Beihang University Collaboration Meeting on Nuclear Physics (University of Tsukuba, Tsukuba, Japan, November 11-12, 2013).

[13] Y. Kuramashi, "Elementary Particle Physics in Future HPC", The 4th AICS International Symposium (RIKEN AICS, Kobe, Japan, December 2-3, 2013).

[14] Y. Kuramashi, "PACS-CS Project and beyond", 新学術領域「素核宇宙融合による計算科学に基づいた重層的物質構造の解明」のまとめと今後を語る研究会 (Narukoonsen, Miyagi, Japan, December 20-21, 2013).

[15] Y. Nakamura, "The critical endpoint in three flavor QCD", Seminar (KEK, Tsukuba, Japan, October 9, 2013).

[16] Y. Nakamura, "The critical endpoint of the finite temperature phase transition in three flavor QCD", Workshop on "Lattice QCD at finite temperature and density" (KEK, Tsukuba, Japan, January 20-22, 2014).

[17] Jarno Rantaharju, "The Gradient Flow Coupling in Technicolor Models", Seminar (Bielefeld University, Bielefeld, Germany, August 13, 2013).

[18] Jarno Rantaharju, "The Gradient Flow Coupling in Technicolor Models", Seminar (University of Helsinki, Department of physics / Helsinki Institute of physics, Helsinki, Finland, August 21, 2013).

[19] Jarno Rantaharju, "Gradient flow coupling schemes in SU(2) with adjoint fermions", JICFuS Mini-workshop on "Gauge theories with many flavors and related topics" (YITP, Kyoto, Japan, March 10, 2013).

[20] Yuya Shimizu, "Analysis of Two-Dimensional Lattice QED in Theta Vacuum using Tensor Renormalization Group", Seminar (Kanazawa University, Kanazawa, Japan, November 15, 2013).

[21] T. Yamazaki, "Calculation of light nuclei in N_f=2+1 lattice QCD", HPCI Field 5 meeting (FUJISOFT AKIBA Plaza, Tokyo, March 3-4, 2014).

[22] Shinji Takeda, "Exploring QCD phase diagram by Wilson type fermions", German-Japanese Seminar (Regensburg, Germany, November 6, 2013).

[23] Shinji Takeda, "Phase structure of finite density QCD", Workshop on "Lattice QCD at finite temperature and density" (KEK, Tsukuba, Japan, January 20-22, 2014).

(4) Posters and Presentations

[24] Y. Kuramashi, "2+1 Flavor Lattice QCD Simulation on K Computer", The 31th International Symposium on Lattice Field Theory (Lattice 2013) (Mainz University, Mainz, Germany, July 29-August 3, 2013).

[25] Y. Nakamura, "The critical endpoint of the finite temperature phase transition for three flavor QCD with clover type fermions", The 31th International Symposium on Lattice Field Theory (Lattice 2013) (Mainz University, Mainz, Germany, July 29-August 3, 2013).

[26] Y. Nakamura, "Towards high performance Lattice QCD simulations on Exascale computers", The International Conference for High Performance Computing, Networking, Storage and Analysis (SC13) (Denver, CO, USA, November 17-22, 2013).

[27] H. Suno, Y. Nakamura, K.-I. Ishikawa, and Y. Kuramashi, "Block BiCGSTAB for lattice QCD on

the K computer", The 4th AICS International Symposium (RIKEN AICS, Kobe, Japan, December 2-3, 2013).

[28] H. Suno, "Theoretical study of weakly bound triatomic systems", JPS 2014 Annual Meeting (Tokai University, Hiratsuka, Japan, March 27-30, 2014).

[29] Xiao-Yong Jin, Yoshinobu Kuramashi, Yoshifumi Nakamura, Shinji Takeda, and Akira Ukawa, "Results from combining ensembles at several values of chemical potential", The 31th International Symposium on Lattice Field Theory (Lattice 2013) (Mainz University, Mainz, Germany, July 29-August 3, 2013).

[30] Jarno Rantaharju, "The Gradient Flow Coupling in Minimal Walking Technicolor", The 31th International Symposium on Lattice Field Theory (Lattice 2013) (Mainz University, Mainz, Germany, July 29-August 3, 2013).

[31] Jarno Rantaharju, "The Gradient Flow and the Running Coupling", Sakata Memorial KMI Mini-Workshop on "Strong Coupling Gauge Theories Beyond the Standard Model" (SCGT14Mini) (Nagoya University, Nagoya, Japan, March 5-7, 2014).

[32] Yuya Shimizu, "An Application of Grassmann Tensor Renormalization Group to Low Dimensional Lattice Gauge Theory", JPS 2014 Annual Meeting (Tokai University, Hiratsuka, Japan, March 27-30, 2014).

[33] Shinji Takeda, "Finite size scaling for 3 and 4-flavor QCD with finite chemical potential", The 31th International Symposium on Lattice Field Theory (Lattice 2013) (Mainz University, Mainz, Germany, July 29-August 3, 2013).

[34] Shinji Takeda, "Exploring finite density QCD with Nf=3 and 4 by Wilson type fermions", The 11th XQCD 2013 (Bern University, Bern, Switzerland, August 5-7, 2013).

Discrete-Event Simulation Research Team

1. Team members

Nobuyasu Ito (Team Leader)

Hajime Inaoka(Research Scientist)

Yohsuke Murase(Research Scientist)

Tetsuo Imai (Postdoctoral Researcher)

Takeshi Uchitane (Postdoctoral Researcher)

Yuta Asano (Postdoctoral Researcher)

2. Research Activities

Development of a management tool for simulations and analyses was started and a prototype is made in this fiscal year of 2013. It is named OACIS (**O**rganizing **A**ssistant for **C**omprehensive and **I**nteractive **S**imulations). It is developed using Ruby, Ruby-on-rail framework and MongoDB. After installation, users register their applications for simulations and analyses, and their computers from PC to supercomputers like K to the OACIS. Then they can design and order executions of simulations and analyses on its web-browser front end. The ssh connection is used to operate the registered remote computers and Job states are supervised by the OACIS. Current prototype transfers output files of simulations and analysis to the local computer operating the OACIS from remote computers. The results and historical data are preserved in local computer using MongoDB.

Algorithm and coding technology of graph and network simulations and analyses are studied. K-oriented program for a benchmark problem, GRAPH500, is designed and developed, although the current version requires further tuning to reach the current world record. An application of agent-based automobile traffic simulation, named MATES developed in the University of Tokyo, is ported to K computer. The MATES is one of few applications of traffic simulation parallelized and coded with C++, and these features are favorable to K computer.

Using the OACIS and the MATES, and an optimization for signal control for a city traffic was performed. A simple GA method coding signal timing is used and traffic simulation using the MATES was executed for each genotype. Signal timing showing shorter averaged travel time was found.

3. Research Results and Achievements

Computers, especially supercomputers nowadays, have been extending the human abilities and possibilities. The frontiers are both in quantity and in quality, which correspond to accuracy and complexity, respectively. DESRT is challenging the latter with the K computer. With the K-class computer, the social activities, which comprise the ultimate of complex phenomena, are in scope of computer applications, and as a matter of course, social modeling and simulations are an objective of DESRT activity.

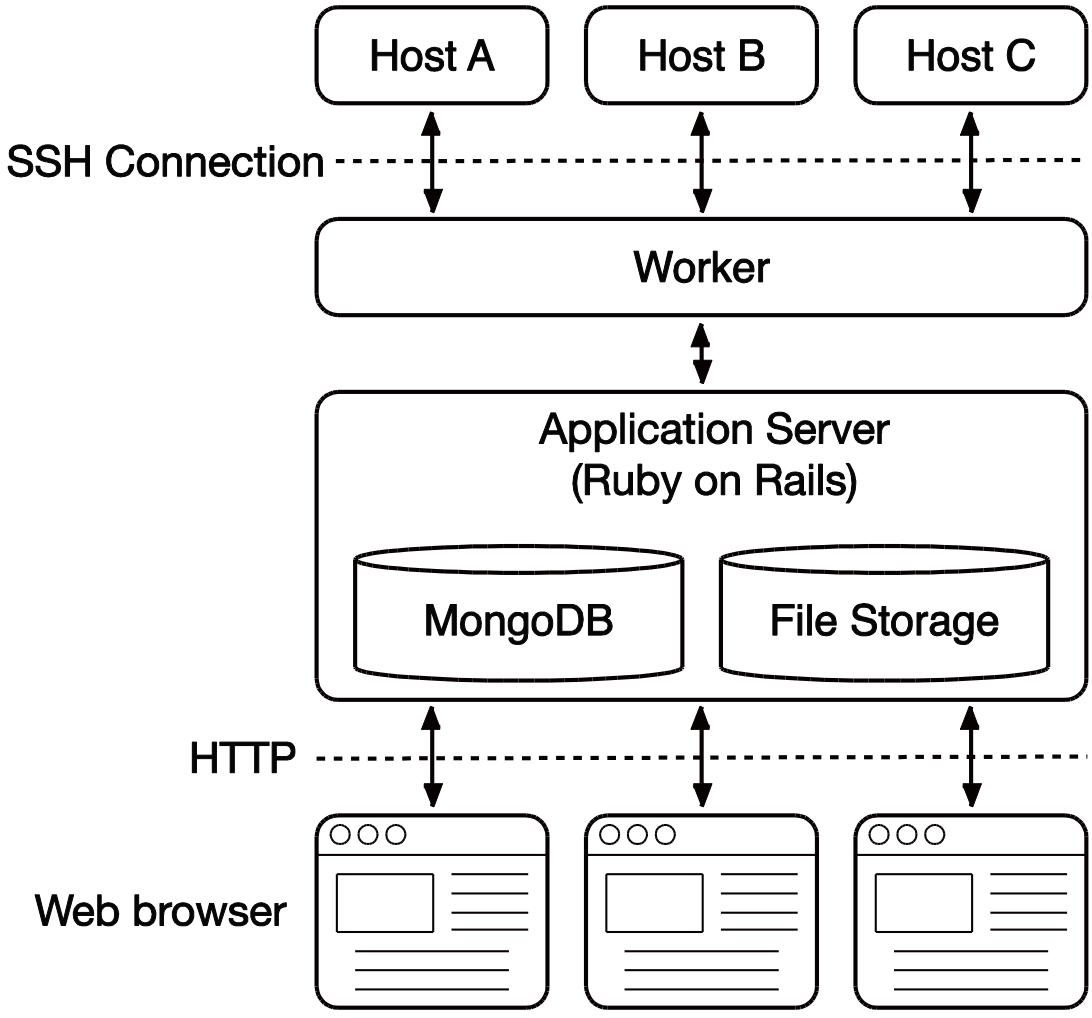
Social modeling has been pursued for long times and the history will be regarded as long as one of human communities. Actually, idea and system of scientific laws of natural phenomena stems from social one like the Roman law. Communities and societies are based on individual people or agents. Small communities and societies with tens people, perhaps, will be managed and controlled based on person-wise or agent-based optimizations, but agent modeling for cities and countries with millions of people and global society with billions of people is not well established yet. In addition to a reliable model, design and optimization with computer simulations requires search for the better parameters, and social parameters usually have discrete option, not analytic nor continuous: a traffic signal is blue or red or some other, and a decision is to adopt an idea or to dismiss it. Therefore a combinatorial complexity is abundant in social application.

A working hypothesis of social application of K-class computer will be to test many kinds of social models, and to challenge their combinatorial possibilities, using huge number of processors. With this hypothesis, the DESRT has been challenging development of a management tool for simulations and analyses, and algorithm and coding technology of graph and network simulations and analyses.

3.1. A management tool for simulations and analyses: OACIS

K-class compuers allow us to execute millions of difference simulations simultaneously, and such big parameter paralellization is an advantage of top-end supercomputers nowaday. But job management by human hands are quite behind the current number of parallelism. We need an efficient intelligent tool to manage such parameter paralellism. If paralellized parameters are quite simple like seed numers for random number generation, such paralellism will be rather easy, although the big nmber itself usually cause sometimes unfeasible operations of comoputers. To overcome the difficulty, the DESRT has been proposing an intelligent application to help to manage the situation. A prototype software tool named OACIS (**O**rganizing **A**ssistant for **C**omprehensive and **I**nteractive **S**imulations) has developed in this year. It is developed using Ruby, Ruby-on-rail framework and MongoDB. After installation, users

register their applications for simulations and analyses, and their computers from PC to supercomputers like K to the OACIS. Then they can design and order executions of simulations and analyses on its web-browser front end. The ssh connection is used to operate the registered remote computers and Job states are supervised by the OACIS. Current prototype transfers output files of simulations and analysis to the local computer operating the OACIS from remote computers. The results and historical data are preserved in local computer using MongoDB.

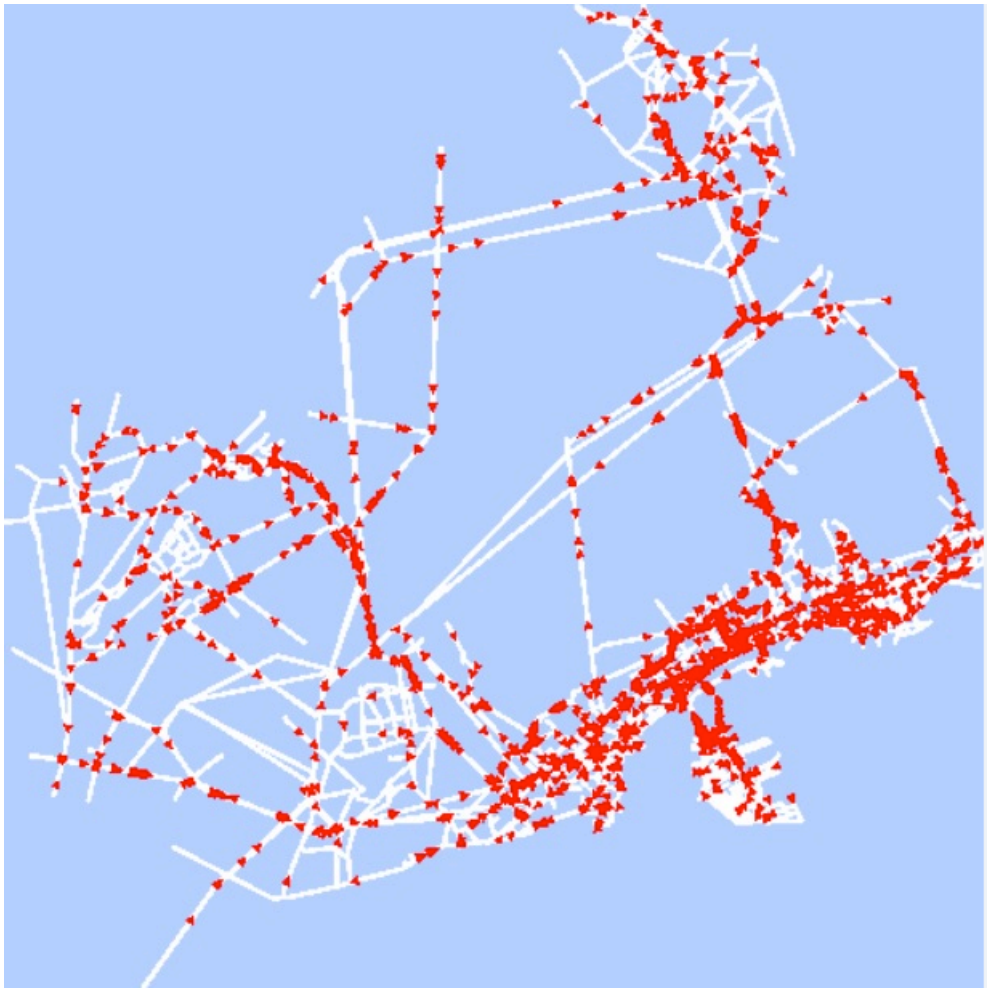


Structure of OACIS is shown schematically.

3.2. Algorithm and coding technology of graph and network simulations and analyses

Algorithm and coding technology of graph and network simulations and analyses are studied. K-oriented program for a benchmark problem, GRAPH500, is designed and developed, although the current version requires further tuning to reach the current world record. An application of agent-based automobile traffic simulation, named MATES developed in the University of Tokyo,

is ported to K computer. The MATES is one of few applications of traffic simulation parallelized and coded with C++, and these features are favorable to K computer.



An example of automobile traffic simulation of the Kobe city.

4. Schedule and Future Plan

In the following years, a beta version of the OACIS is released to the public, and tools of visualization and simulation design will be developed. And a graph simulation and analysis tool working on K-computer up to its full node will be developed.

Computational Molecular Science Research Team

1. Team members

Takahito Nakajima (Team Leader)
Yutaka Imamura (Research Scientist)
Tomomi Shimazaki (Research Scientist)
Yoshinobu Akinaga (Research Scientist)
Michio Katouda (Postdoctoral Researcher)
Yutaka Nakatsuka (Postdoctoral Researcher)
Taichi Kosugi (Postdoctoral Researcher)
Toru Matsui (Visiting Researcher)
Muneaki Kamiya (Visiting Researcher)

2. Research Activities

Developing a Molecular Theory and Software for Predicting Reactions and Properties of Molecules

2.1. Employing original theory-based calculations to develop new materials and drugs

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.

2.2. New software makes best possible use of the processing power of the K computer

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.

3. Research Results and Achievements

3.1. Development and application of computation methods for accurate treatment of non-covalent bonding interaction of nano-scale supermolecules

Non-covalent bonding interactions often take very important roles for structural and thermochemical properties of nano-materials such as the self-assembly of supermolecules. Analysis applying robust theoretical and computational approach has been desired for the elucidation and reliable prediction of non-covalent bonding interactions in nano-scale supermolecules. Last year, we developed the MPI/OpenMP hybrid parallel algorithm and its code for the massively parallel computations of the resolution-of-identity second-order Møller–Plesset perturbation (RI-MP2) method. This algorithm works efficiently on not only commodity supercomputers such as the RIKEN RICC massively parallel PC cluster system but also the K computer. Using the new parallel RI-MP2 code, MP2 calculations of large molecules having up to 500 atoms and 10,000 atomic orbitals can be performed with high parallel performance and in modest times on K computer. In this year, we developed a code for the massively parallel computation of the double-hybrid density functional theory (DH-DFT) based on the parallel RI-MP2 code. Using the parallel RI-MP2 and DH-DFT code, we assessed the performance for π–π stacking interaction energy of two-layer nanographene sheets $(C_{24}H_{12})_2$, $(C_{54}H_{18})_2$, $(C_{96}H_{24})_2$, and $(C_{150}H_{30})_2$ at the MP2, SCS-MP2, and B2-PLYP-D3 levels with the cc-pVTZ basis set. We successfully performed the RI-SCS-MP2/cc-pVTZ calculation of $(C_{150}H_{30})_2$ (9,840 atomic orbitals) on 8,911 node and 71,288 CPU cores of K computer in 65 minutes. The results demonstrate that reliability of SCS-MP2, and B2-PLYP-D3 for the accurate calculations of the π–π stacking interaction energy: SCS-MP2 and B2-PLYP-D3 give similar results and well reproduce the experimental results while MP2 gives overestimation of results. We have also been developing the parallel RI-MP2 analytical energy gradient algorithm and its code enable to perform the geometry optimization calculations of nano-molecules with about 500 atoms on the K computer.

3.2. Application of two-component relativistic coupled-cluster programs

Consideration of relativity in molecular quantum-chemical calculations is one of the most important factors for heavy-element systems. In 2011 we developed general-order spin-free and two-component relativistic spin–orbit coupled-cluster (SOCC) programs for ground- and excited-state correlation energies with the aid of an automatic code-generation technique. The developed generator program derives algebraic CC equations automatically for a given order, factorizes the terms in each equation, and generates Fortran programs for solving the equations. The development in 2012 includes improvement of the generator such that level 3 BLAS routines are used, automatic algebraic derivation and solution of Lambda equations, and IP-EOM (ionization potential equation-of-motion) CC equations with both spin-free and spin–orbit formalism. In this period we applied the developed method to excitation energies, potential energy curves, and ionization potentials of molecules. Excellent agreement was obtained between the calculated results using our programs and experiment for the ionization spectrum of an OsO_4 molecule, which is known to exhibit a well-known splitting due to spin–orbit interaction. The potential energy curves are computed for ground- and excited states of TlH molecule in the level of spin–orbit EOM-CCSDT (Figure). Inclusion of full triple excitations results to the correct behavior of potential energy curves with long interatomic distances. Correct level splittings are predicted owing to inclusion of spin–orbit interaction.

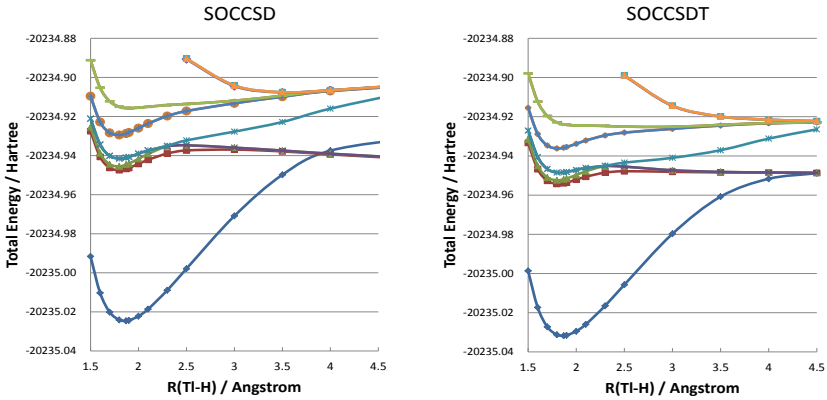


Figure: Potential energy curves of TlH at SO-CCSD and SO-CCSDT levels of theory

3.3 Development of two-component relativistic time-dependent density functional theory program with spin–orbit interaction

The inclusion of relativity is crucial for a proper description of photochemistry for systems containing heavy elements. In particular, it is known that spin–orbit coupling affects excited-state characters, relaxation dynamics, radiative and non-radiative decay pathways, as well as lifetimes and reactivity. Time-dependent density functional theory (TDDFT) has become one of the most widely used methodologies for computing excited states because of its reasonable cost and relatively high accuracy. Until now, in almost all the TDDFT calculations for

heavy-element systems, only the scalar relativistic effect was taken into account while the spin-orbit coupling effect on the excitation energies was not considered. In this work, we have implemented the two-component relativistic TDDFT with spin–orbit interaction method in the NTChem programs. Our implementation is based on a noncollinear exchange–correlation potential presented by Wang et al. This formalism is suitable in relativistic TDDFT calculations with spin–orbit coupling and has the correct nonrelativistic limit and recovers the correct threefold degeneracy of triplet excitations for closed-shell systems. The matrix elements of the noncollinear exchange–correlation kernel have been derived and implemented into efficient computer codes with the aid of a newly-developed computerized symbolic algebra system. In addition, various DFT functionals including the recently proposed range-separated hybrid functionals are applicable to the calculations of excitation energy for spin–orbit coupled states.

3.4. Development of ASEP/MM for inclusion of solvent effects

The solvent effect is important in considering the relation between experimental and computational results. To investigate the effect of solvent over solute electronic structure, several methods have been proposed such as the polarizable continuum model, the reference interaction site model, and so on. We have implemented the averaged solvent electrostatic potential (ASEP) scheme in the NTChem program. The ASEP/MD scheme is a kind of the quantum mechanics/molecular mechanics (QM/MM) method, where the solvent molecule is treated in the MM calculation with the fixed solute charges and introduced in the QM calculation of solute atom in the averaged fashion. The QM and MM calculations are performed iteratively until the whole convergence. In our implementation, Tinker, which a free MM code developed in Jay Ponder group, is adopted as the MM calculation code and the iterative QM/MM cycle is built in the SCF part of the NTChem program, and users can perform ASEP/MM calculation without a cumbersome manual operation of the QM/MM iteration. The energy and gradient calculations using the ASEP/MD scheme are now available.

3.5. Development of advanced QM/MM MFEP code for supramolecules

Supramolecules (host) which contain a vacant space can contain other small molecules (guest) in the inner space, and this host–guest type complex often shows an unusual stability of a guest molecule or a characteristic reactivity. In these systems, the host molecule offers the reaction space and is supposed to interact with the included guest molecule quantum mechanically in the specific site and molecular mechanically in the remaining sites. Thus, it seems to be necessary that the host–guest reaction is investigated by the free-energy analysis. We have developed an extension of QM/MM MFEP of Hu et al. to include the guest–host QM interaction via the QM calculation of whole system and the temperature dependent interaction via the QM/MM molecular dynamics simulation. This scheme is derived from the full QM free energy

expression and the temperature dependent part is approximated with QM/MM scheme. The developed extended QM/MM MFEP scheme is implemented in the NTChem program and applied to the Diels–Alder reaction in the supramolecule. In the single point calculation for the enthalpy based Diels–Alder reaction path, the reaction barrier of the free-energy is 15.5 kcal/mol whereas the reaction barrier of the enthalpy is 28.4 kcal/mol. This result shows the dynamical motion of host molecule decrease the reaction barrier of the guest molecule.

3.6. Development of the range-separation density-fitting approach for first-principles-based material quantum chemistry

First-principles quantum chemistry methods are widely used in science and engineering, and in recent years they have been employed to investigate various materials, such as polymers, semiconductors, surface and interface systems, and bulk materials. For example, first-principles quantum chemistry methods can be used to accelerate the development of solar cells and solid catalytic systems, which are expected to contribute to solving energy and environmental problems. Thus, material quantum chemistry, which is quantum chemistry for the development of materials, is important. The electronic structure calculation under the periodic boundary conditions (PBCs) is an essential tool for material quantum chemistry. Therefore, we have developed a range-separation density-fitting method for obtaining the electronic band structure under periodic boundary conditions. The Hartree term and the nuclear attractive term are divided into long- and short-range contributions by using the error and complementary error functions, respectively. In the method, the long-range Hartree term is evaluated through a density-fitting procedure based on Gaussian auxiliary functions, where the net charge neutrality of electrons and atomic nuclei in the unit cell is ensured by Lagrange multipliers. We checked our method using the energy band structures of a two-dimensional monolayer sheet (graphene) and a three-dimensional periodic system (diamond) based on both semi-local density functional theory (DFT) functionals and the Hartree–Fock and hybrid DFT methods. From those calculations, we confirmed our method is suitable for investigating the electronic structure of materials under the PBCs. In these calculations, we also confirmed that the range-separation approach can yield good electronic structure descriptions, especially in interconnection between short- and long-range Hartree terms, because of expressive Gaussian auxiliary functions. On the other hand, the long-range contribution of the Hartree term needs much smaller CPU time than the short-range contribution, because the short-range Hartree term is estimated from heavy four-center electron-electron repulsive integrals, and thus the calculation cost to employ Gaussian auxiliary functions do not have disadvantages on the total calculation time. We only examine the basic calculations at present, and will apply the method to some important materials in the near future.

3.7. Development and implementation of a new exchange correlation functional for electronic structure calculations of periodic systems

First-principles calculations of electronic structures based on density functional theory (DFT) are today recognized as one of the most powerful tools for analyses and predictions of various properties of electronic systems. Some DFT functionals proposed so far were thus constructed to reproduce the results of numerical calculations such as quantum Monte Carlo simulations of a free-electron gas. We adopted another approach to construct a DFT functional based on the spirit of the Hedin's GW theory. The GW theory is described by the system of integral equations on the basis of the Green's function theory for a many-body electronic system, which provides electronic band structures exhibiting good agreement with the experimental ones, especially for semiconductors. We adopted a model dielectric function to construct an exchange correlation functional starting from the screened Coulomb potential. Furthermore, the Coulomb-hole interaction term was added. Such an approach has not been reported so far, to our best knowledge. Our approach may thus give insights into the relation between DFT functionals and the many-body theory based on the Green's function. We found for the various semiconductors that the calculated band gaps with the new functional are closer to the experimental values than those with the PZ81 functional are. The optimal bulk properties of the semiconductors were also examined, and we confirmed the new functional can give comparable calculation results as the PZ81 functional. These calculations corroborate the validity of our approach.

3.8. A computational approach to the selectivity of nucleobase in supramolecular cage

We investigated the mechanism of the conformation selectivity of adenine–uracil (AU) pair in supramolecular cage from the view of computational chemistry. We used a program package "NTChem" which enables us to perform a molecular calculation by a massively parallel multi-core supercomputer such as the K computer. Judging from the optimized geometry shown in the right figure, N3 of adenine and O4 of uracil mainly contribute to the broadening π orbitals and interact with pyridines in the case of anti-Hoogsteen (AH) type. When applied relativistic effect, the volume of molecular cage becomes smaller because the bond length Pt–N gets smaller in 0.1 Å and strengthens the vdW interaction between AU pair and molecular cage.

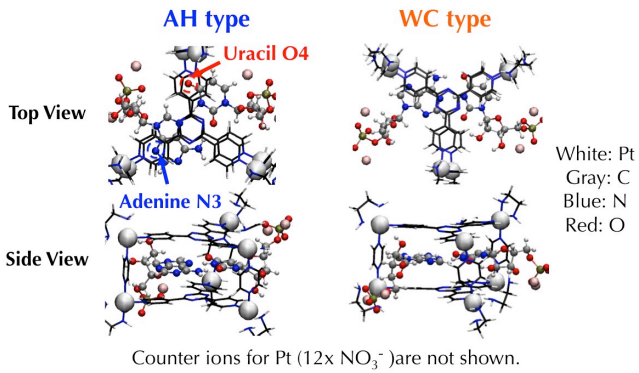


Figure: Optimized geometries of AU pair in supramolecular cage.

According to the result of maximally interaction orbital (MIO) analyses, there exists a CH/π interaction between C5–H of uracil and a side of supramolecular cage, which stabilizes the whole structure rather than Watson–Crick type.

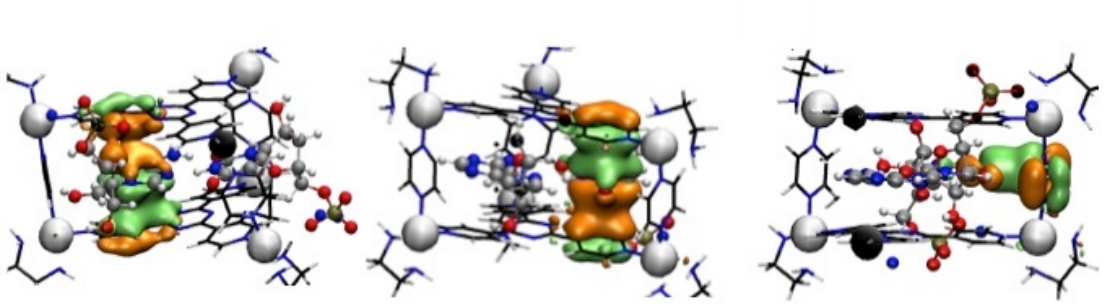


Figure: The most contributing molecular orbitals to stabilizing the AH type. (a), (b) π–π interaction between Au pair and cage. (c) CH/π interaction, seen in only AH type.

3.9. Theoretical study on a new dye-sensitizer, DX1 molecule by time-dependent density functional theory with spin–orbit interaction

Ru complexes have been demonstrated as a promising dye for a few decades. Recently, a phosphine-coordinated Ru(II) sensitizer, DX1 molecule, was reported to generate the highest value for an organic photovoltaic. The DX1 molecule has the feature that spin-forbidden singlet-to-triplet direct transitions occur because of the strong spin–orbit (SO) interaction, which indicates that the new DX1 sensitizer can avoid energy loss originating from intersystem crossing. In order to examine the spin-forbidden transitions in details, this study calculates the transition energies by two-component relativistic time-dependent density functional theory (TDDFT) with SO interaction, which was based on Tamm–Dancoff approximation (TDA) and was implemented into the quantum chemical program package, NTChem. The singlet-to-triplet transition around 1.3 eV, which is assigned to a metal-to-ligand charge-transfer type excitation, appears although it is slightly shifted to a lower energy in comparison with the experimental spectrum, probably due to lack of solvation effect. The major other peaks in the energy range from 1.5 to 3.0 eV are also reasonably reproduced with the tendency of the slight underestimation. Thus, this study confirms that two-component relativistic TDDFT/TDA calculations can reproduce spin-forbidden singlet-to-triplet transitions with reasonable accuracy. Also, the lowest peak observed for the absorption spectra of DX1 molecule is assigned to the singlet-to-triplet direct spin-forbidden transition.

4. Schedule and Future Plan

In the next financial year, we will improve the parallel efficiency of the NTChem2013 suit of program which was released on the K computer in this fiscal year. In addition, we will make

NTChem more user-friendly. We intend to continue adopting users' requests with the aim of making it more convenient and usable for researchers in many fields. We expect that NTChem will enable, for example, researchers to predict the structures of biological molecules as they relate to drug actions, and to elucidate the mechanisms by which nano-materials exhibit their unique functions.

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] T. Nakajima, "Douglas–Kroll method", *Journal of Computer Chemistry, Japan*, **13**, 50–70 (2014). (in Japanese)

[2] K. Uehara, T. Miyachi, T. Nakajima, N. Mizuno, "Effect of Heteroatoms on Electronic States of Divanadium-Substituted γ-Keggin-type Polyoxometalates", *Inorg. Chem.*, in press.

[3] T. Shimazaki, T. Kosugi, T. Nakajima, *J. Phys. Soc. Jpn.*, in press.

[4] R. Sakanoi, T. Shimazaki, J. Xu, Y. Higuchi, N. Ozawa, K. Sato, T. Hashida, M. Kubo, "Different Behavior of Young's Modulus and Fracture Strength of CeO_2: Density Functional Calculation", *J. Chem. Phys.*, in press.

[5] T. Kosugi, "Repeated Extraction of Work via Measurements on Nonequilibrium Two Particles Interacting in a Harmonic Trap", *J. Phys. Soc. Jpn.* **83**, 054001 (2014).

[6] T. Kosugi, T. Miyake, S. Ishibashi, "Second-order Perturbation Formula for Magnetocrystalline Anisotropy using Orbital Angular Momentum Matrix", *J. Phys. Soc. Jpn.* **83**, 044707 (2014).

[7] S. Akamaru, T. Shimazaki, M. Kubo, T. Abe, "Density functional theory analysis of methanation reaction of CO_2 on Ru nanoparticle supported on TiO_2 (101)", *Applied Catalysis A*, **470**, 405 (2014).

[8] M. Katouda, T. Nakajima, "MPI/OpenMP hybrid parallel algorithm of resolution of identity second-order Møller–Plesset perturbation calculation for massively parallel multicore supercomputers", *J. Chem. Theory Comput.* **9**, 5373–5380 (2013).

[9] T. Kosugi, "Perpetual extraction of work from a nonequilibrium dynamical system under Markovian feedback control", *Phys. Rev.* E **88**, 032144 (2013).

(2) Invited Talks

[10] T. Nakajima, "NTChem for photosynthesis", Symposium for photosynthesis, Kobe, 8 Mar. 2014. (in Japanese)

[11] T. Nakajima, "NTChem", Supercomputer workshop 2014, Okazaki, 21 Jan. 2014. (in Japanese)

[12] M. Katouda, T. Nakajima, "MPI/OpenMP hybrid parallel algorithm of resolution of identity second-order Møller–Plesset perturbation calculation for K computer", 5th JCS International Symposium on Theoretical Chemistry, Nara, 4 Dec. 2013. (Poster)

[13] T. Shimazaki, T. Kosugi, T. Nakajima, "Development of first-principles calculation method under periodic boundary condition for material quantum chemistry", 5th JCS International Symposium on Theoretical Chemistry, Nara, 4 Dec. 2013. (Poster)

[14] Y. Imamura, M. Kamiya, T. Nakajima, "Two-component Relativistic Time-dependent Density Functional Theory: Development and Applications", 5th JCS International Symposium on Theoretical Chemistry, Nara, 4 Dec. 2013. (Poster)

[15] T. Nakajima, "NTChem for chemical reaction", "New frontier for chemical reaction", Kyoto, 28 Sep. 2013. (in Japanese)

[16] T. Nakajima, "NTChem and K computer", TCCI symposium, Okazaki, 10 Sep. 2013. (in Japanese)

[17] T. Nakajima, "NTChem: A High-Performance Software Package for Molecular Electronic Structure Calculation on K Computer", 6th Asia-Pacific Conference on Theoretical & Computational Chemistry, Gyeongju, 11 Jul. 2013.

(3) Posters and Presentations

[18] T. Matsui, T. Nakajima, "pKa Estimation for Side Chain of Amino Acid in Protein", the 94th Annual meeting of Chemical Society of Japan, Nagoya, Japan, 27 Mar. 2014. (in Japanese)

[19] T. Nakajima, "NTChem: A High-Performance Software Package for Molecular Electronic Structure Calculation", CMSI・SPring-8・J-PARC・KEK symposium 2014, Kashiwa, March, 2014. (Poster in Japanese)

[20] T. Matsui, T. Nakajima, "A Computational Approach to the Selectivity of Nucleic Acid in Supramolecular Cage", The 63rd Conference of Japan Society of Coordination Chemistry, 3 Nov. 2013. (Poster in Japanese)

[21] T. Nakajima, "NTChem: A High-Performance Software Package for Molecular Electronic Structure Calculation", 7th Annual Meeting of Japan Society for Molecular Science, Kyoto, Japan, Sep. 2013. (in Japanese)

[22] T. Matsui, T. Nakajima, "A Theoretical Study on the Redox Potential of metallothioneins", 7th Annual Meeting of Japan Society for Molecular Science, Kyoto, Japan, 27 Sep. 2013. (Poster in Japanese)

[23] M. Kamiya, T. Nakajima, "Development of analytical energy gradient for two-component relativistic time-dependent density functional theory", 7th Annual Meeting of Japan Society for Molecular Science, Kyoto, Japan, Sep. 2013. (Poster in Japanese)

[24] T. Shimazaki, T. Kosugi, T. Nakajima, "Development of ab-initio calculation method under periodic boundary conditions for material quantum chemistry", Anuual Meeting of Japan Society for Molecular Science (2013), Kyoto, 24 Sep. 2013. (in Japanese)

[25] Y. Akinaga, T. Nakajima, "Development of two-component relativistic coupled-cluster methods: application to molecular ground and excited states", 7th Annual Meeting of Japan

Society for Molecular Science, Kyoto, Japan, Sep. 2013. (Poster in Japanese)

[26] M. Katouda, T. Nakajima, "Development of MPI/OpenMP hybrid parallel algorithm of resolution of identity second-order Møller–Plesset perturbation calculations for massively parallel multicore supercomputers", ISTCP-VIII, Budapest, Hungary, 29 Aug. 2013. (Poster)

[27] Y. Nakatsuka, T. Nakajima, "Development of Relativistic quantum Monte Carlo method: Theory and parallel program", ISTCP-VIII, Budapest, Aug. 2013. (Poster)

[28] M. Katouda, T. Nakajima, "Analysis of π–π interaction of nanographene surfaces using MP2 method and dispersion corrected DFT", 16th Theoretical Chemistry Symposium, Fukuoka, Japan, 16 May 2013. (Poster in Japanese)

(4) Patents and Deliverables

[29] NTChem2013, released on 29 Aug. 2013.

Computational Materials Science Research Team

1. Team members

Seiji Yunoki (Team Leader)

Yuichi Otsuka (Research Scientist)

Shigetoshi Sota (Research Associate)

Shixun Zhang (Postdoctoral Researcher)

Sandro Sorella (Senior Visiting Researcher)

Yoko Hosokawa (Assistant)

2. Research Activities

The computational materials science research team focuses mainly on the following subjects:

1. We develop a quantum Monte Carlo (QMC) method, which is one of the most reliable and efficient techniques for a Hubbard-type lattice model of interacting electrons. Typical target systems we aim are of the order of 10,000 electrons unless the notorious minus-sign problem occurs.
2. We develop a massively parallelized two-dimensional (2D) density matrix renormalization group (2-D DMRG) algorithm to investigate two-dimensional strongly correlated quantum systems on K computer. Although 2-D DMRG method requires huge computational costs, this method is thus far one of the most effective schemes to study 2D strongly correlated quantum systems. Our developed massively parallelized 2-D DMRG algorithm enables us to perform the calculations for large system sizes with high accuracy.
3. We develop a Monte Carlo (MC) method for systems where electrons are coupled to classical degrees of freedom, e.g., a system described by the double exchange (DE) model, to simulate complex magnetic structures such as Skyrmions. As we have to evaluate very frequently the eigenvalues of a given Hamiltonian to eliminate the electronic degree of freedom, we seek the highly efficient implementation and optimization of novel numerical methods and algorithms with low time complexity and therefore large system sizes can be reached. For example, using the kernel polynomial method, we develop an O(*N*) Green-function-based MC (GFBMC) method.

3. Research Results and Achievements

3.1. QMC simulations for metal-insulator transitions in Dirac fermions

We have implemented a highly efficient QMC code based on the auxiliary filed scheme for lattice fermion systems at zero temperature. Since numerical calculations involved in this formulation are mostly linear algebraic procedure such as matrix-matrix product and numerical

orthogonalization, we can take advantage of the highly optimized numerical library on K computer to calculate physical observables with a high degree of accuracy on quite large systems.

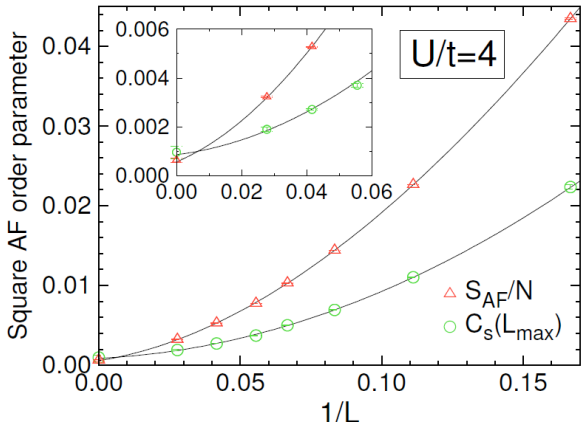


Fig. 1. Extrapolations to the thermodynamic limit of squared AF order parameter at U/t=4. S_{AF} is the AF spin structure factors and $Cs(L_{max})$ is the spin-spin correlation functions at the maximum distance.

First, we have applied this improved code to elucidate the ground state phase diagram of the half-filled Hubbard model on the honeycomb lattice model, in which a gapped spin liquid (SL) phase have been predicted [Meng et al., *Nature* 464, 847 (2010)]. Since it is widely believed that not only strong quantum fluctuations but also geometrical frustrations are responsible for stabilizing SL phase, the finding of SL phase in the unfrustrated honeycomb lattice is rather surprising, and thus has been one of the most debated issues in recent years. The possible SL phase in the previous report has been claimed to exist for $3.4 < U/t < 4.3$ (U/t: measure of the Hubbard interaction) as a spin-gapped insulating phase without any broken symmetry. We thus have first tried to clarify the existence of SL at $U/t = 4$, which corresponds to the middle of the SL region. Taking a full advantage of K computer, we have performed the QMC simulations on the lattice with size up to N=2,596 sites, currently the largest system size available in the world. Figure 1 shows our results of the AF spin structure factors, S_{AF}, and spin-spin correlation functions at the maximum distance, $Cs(L_{max})$ at $U/t = 4$. The extrapolated values of both quantities are confirmed to be finite within statistical errors, indicating the AF long-range order. Complemented with simulations performed at other U/t, our results strongly support the conventional scenario that a single and direct phase transition occurs between semi-metal (SM) and antiferromagnetic Mott insulator (AFMI) with increasing U/t: Absence of the spin liquid.

Next, we have investigated the Mott transition in the Hubbard model on square lattice with a magnetic flux π per plaquette, where the low-lying excitations at weak coupling are described by massless Dirac fermions. This low-energy electronic dispersion around the Fermi level is very similar to the case of the Hubbard model on the honeycomb lattice, and indeed a SL phase has also been proposed to exist between SM and AFMI [Chang and Scalettar, *Phys. Rev. Lett.* 109, 026404 (2012)], which is claimed as a gapless phase for this model. Our highly developed code and experience obtained in the previous study for the honeycomb lattice, enable us to examine this possibility to have the SL phase also in this model. By performing careful finite-size scaling

for the spin-spin and density-density correlation functions, calculated with a high degree of accuracy, we find that the ground state is likely to be divided into only two regions, paramagnetic SM and AFMI phases, suggesting again the conventional scenario of the single continuous Mott transition.

3.2. Development of massively parallelized 2-D DMRG algorithm

The DMRG procedure is known as one of the most powerful and accurate numerical methods for one-dimensional strongly correlated quantum systems. To the contrary, in the two- or higher spatial dimensional dimensions, the DMRG method has been less accurate because, to obtain the accurate or even reliable physical quantities in higher dimensions, the DMRG method requires an exponentially large DMRG truncation number m, which determines the computational costs (i.e. the dimension of a Hamiltonian is given by m^2). Figure 2 shows the DMRG truncation error and the m dependence of one- and two-dimensional (triangular lattice) Hubbard model. Here, the number of site N=36 for both cases. In the one-dimensional case, we confirm the convergence of the ground energy up to m=50 which is the quite small number of states kept as compared with the full Hilbert space dimension to describe this system. This means that we can obtain accurate ground state of one-dimensional Hubbard model by this small truncation number m. However, in the two dimensional case, we cannot obtain the converged ground energy even up to m=2000. This means that we require much larger m to obtain the accurate result for the two-dimensional case. This is the reason that we require a huge computer system such as K computer to perform the 2-D DMRG method to investigate two-dimensional strongly correlated systems.

In this academic year, we have implemented the efficient memory usage to perform the large m 2-D DMRG calculation on the K-computer. In particular, we have reduced the memory usage of operators at each site. At each DMRG step, the bases sets of all operators are transformed to the new basis set to describe arbitrary target states. Thus we have to keep all operators during the DMRG calculations. Furthermore, in the case of N-body operators, we have to keep all of its combinations, since N-body operators should not be given simply by the multiplication of the transformed one-body operators in the DMRG calculation to keep the accuracy. Thus, the number of operators that we need to perform becomes inevitably very large. In our 2-D DMRG, we employ new algorithm to perform the transformation of the basis set of each operator. In the usual algorithm of the DMRG calculation, all operators are transformed after diagonalizing the reduced density matrix given by the target states. In our case, we perform the transformation of operators when we need for the calculations. Therefore, we keep only the transformation matrices, which are given by the eigenvectors of the reduced density matrices. Thus, the size of memory usage is reduced as compared with the usual cases. Furthermore, the

elapsed time of our DMRG calculation is almost the same, since the elapsed time of the basis transformation is very small as compared with the total elapsed time of the DMRG calculations. Employing our DMRG technique, we can perform simulations for large system sizes with keeping much larger *m*.

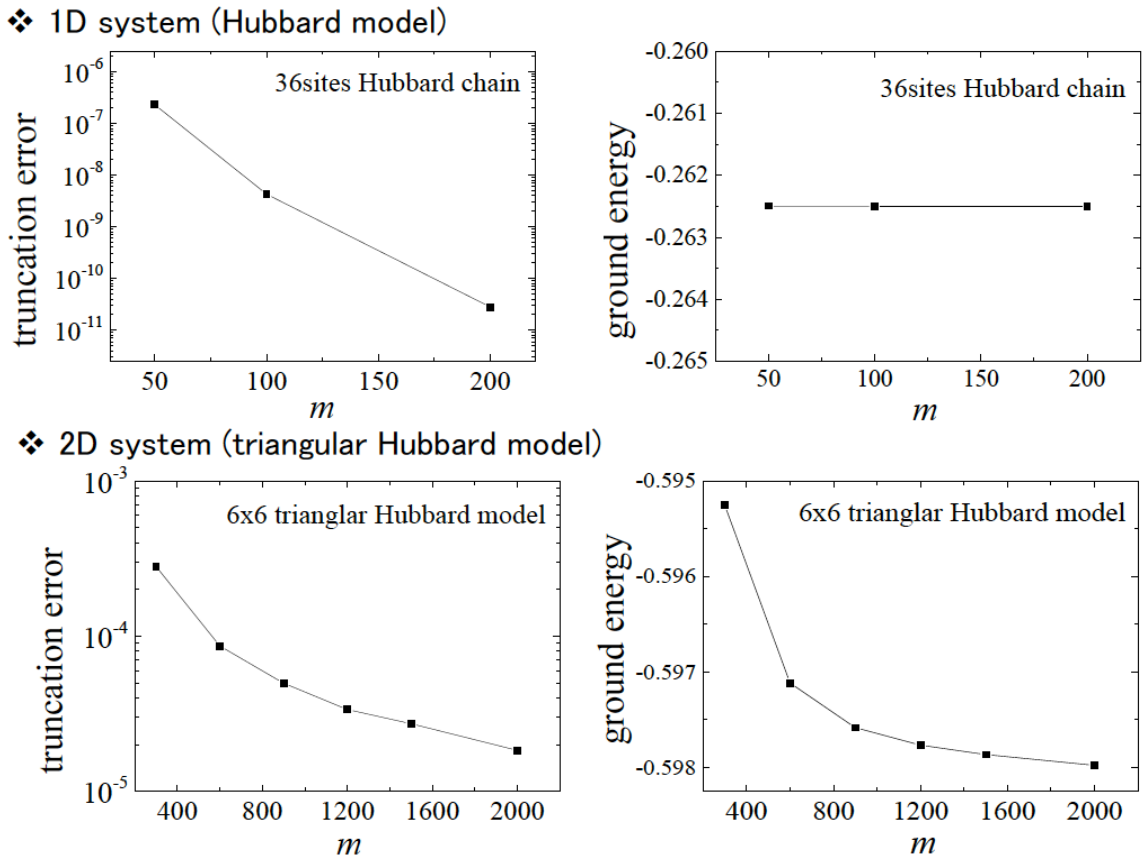


Fig. 2. the DMRG truncation error and the calculated ground state energy as a function of *m* for the one- and two-dimensional (triangular) Hubbard models.

3.3. Time-dependent 2-D DMRG algorithm

The DMRG method has been employed to investigate the time-dependence quantum dynamics for one-dimensional strongly correlated quantum systems by using the Suzuki-Torroter decomposition. However, we cannot employ the same algorithm of the time-dependent DMRG calculation in two dimensions because it is difficult to use the Suzuki-Torroter decomposition. Here, we have developed a new two-dimensional time-dependent 2-D DMRG method by using the kernel polynomial method.

In the DMRG method, the basis set in the limited Hilbert space is optimized to describe arbitrary target states. For example, in the case of the zero temperature calculation, the ground state is

the target state. The target state is now dependent on time. As mentioned above, in one-dimensional systems, the time-evolution of the state is calculated using the Suzuki-Torotter decomposition. In this case, we can perform an efficient calculation of the time-dependent DMRG since we should consider only interactions between added sites. In two-dimensional systems, we employ the kernel polynomial method to obtain the time-evolution of a state. The kernel polynomial method is known as an O(*N*) method. Here, the time-evolution operator is expanded by the kernel polynomial method. As a test calculation, we have investigated the relaxation process of the two-dimensional Heisenberg model. First, we calculate the ground state of the Heisenberg model on the two-dimensional square lattice. Then, we add additional spin exchange interactions between spins located on the diagonal direction of the square lattice, forming the triangular lattice. Note that the ground state of the Heisenberg model on the square lattice is not the ground state (or any eigenstate) of the Heisenberg model on the triangular lattice. Figure 3 demonstrates the relaxation process from the ground state for the square lattice after adding the additional spin exchange interactions to form the triangular lattice, calculated using our time-dependent 2-D DMRG.

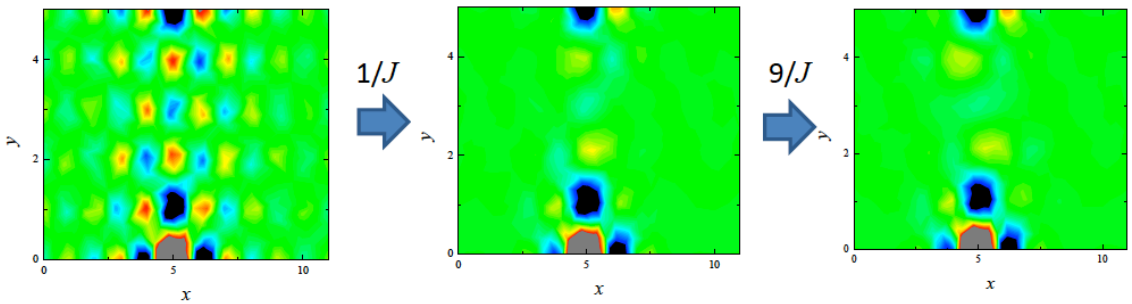


Fig. 3. The time-dimendence of spin-spin correlation functions. The left, center, and right panels show the spin-spin correlation function at time t=0, t=1/J, and t=10/J, respectively.

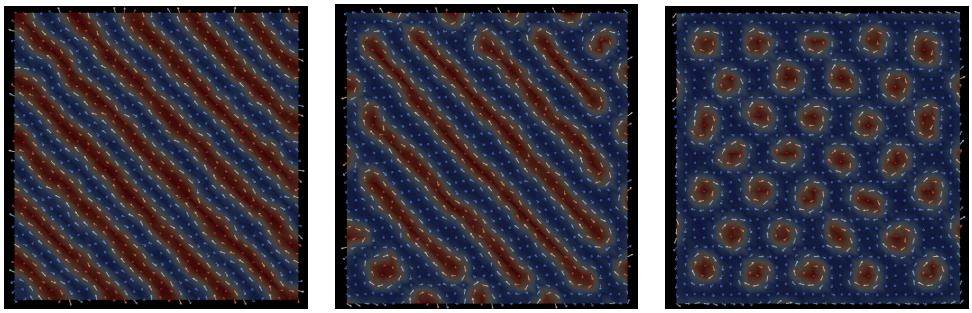
3.4. GFBMC simulations for the DE model and complex magnetic structures

We have first developed the simulation program based on a method using Chebyshev expansion to solve the Green's function of conduction electrons. Instead of numerically exactly diagonalizing, we have adopted the expansion method that exhibits significantly high performance, mainly due to its O(*N*) time complexity. To improve the execution efficiency of the C++ code, we have also performed deep optimizations including rearranging of the memory layout and rewriting the program kernel directly using SIMD instructions.

After successfully implemented the first version of the program that is specially optimized for K computer, we have performed initial simulations for the DE model and confirmed that we can reproduce the results reported in the pervious studies. In addition, as shown below, we have

obtained for the first time the Skyrmion crystal phase in the 2D model that explicitly includes the electron degree of freedom. We have also evaluated the conductivity tensor of conduction electrons in the background of classical spin configuration, and found that the Hall conductivity obtained is in good qualitative agreement with the Skyrmion phase diagram, revealing the topological nature of the Skyrmion.

The DE model is composed of conductive electrons coupled to localized classical spins. Incorporating Dzyaloshinskii-Moriya interaction and magnetic field into the DE model, we have successfully reproduced the complex magnetic structures including helical phase, Skyrmion crystal phase, and ferromagnetic phase on the 2D square lattice. As shown in Fig 4, with increasing a magnetic field, the system goes through from the helical phase, which feathers the strip-style formation of spins with same direction, to the Skyrmion crystal phase in which Skyrmions are crystalized in a hexagonal lattice.



$B=0$ $B=0.09t$ $B=0.13t$

Fig 4. Magnetic field dependance of Skyrmion on 2D 32×32 lattice. The magnetic filed B is indicated in the figures. t is the hopping of the conduction electrons.

We have also examined the conductivity tensor evaluated using Kubo's formula. Due to the topological nature of Skyrmions, the electrons moving through Skyrmions will collect Berry's phase, which can be treated as a source of emergent electromagnetic field (EEF). In this case, it is expected that the EEF affects the motion of electrons and thus induces non zero Hall conductivity. We have found that our numerical results support this expectation and are in good qualitative agreement with experimental observation.

4. Schedule and Future Plan

4.1. QMC simulations for metal-insulator transitions in Dirac fermions

In the course of our studies for Dirac fermions, we have noticed that the Mott transitions in both cases, on the honeycomb lattice with no flux and on the square lattice with π-flux, are likely to be governed by the same universality class. To clarify this unique phenomenon, we plan to calculate critical exponents for the Mott transitions with even higher accuracy using even

larger lattice sizes. It is noted that the Mott transition in Dirac fermions has a close relation to quantum transitions in three-dimensional lattice Gross-Neveu models discussed in particle physics. We thus believe that our results will be of general interest in a wide range of research field. To perform the simulations for larger system sizes on K computer, we will keep developing a new algorithm to share a single Slater determinant with multiple nodes.

4.2. 2-D DMRG simulations for strongly correlated quantum systems

Using our massively parallelized 2-D DMRG, we will investigate properties of various kinds of strongly correlated quantum systems, including a metal-insulator transition for the half-filled Hubbard model on the triangular model, magnetic order phases on the Kitaev-Heisenberg model on the honeycomb lattice, a possible superconducting phase on the Hubbard model on the square lattice, dynamical properties for various optical lattice systems, a possible spin liquid phase of the anisotropic Heisenberg model on the triangular lattice, and photo-induced phase transition and quantum relaxation processes of the strongly correlated quantum systems. As an implementation of our 2-D DMRG, we will develop a dynamical 2-D DMRG and a finite temperature 2-D DMRG.

4.3. MC simulations for electrons coupled to classical degrees of freedom

We will continue to develop massively parallelized O(N) GFBMC that is optimized on K computer. To efficiently simulate a system as large as 10,000 sites, we still need to further optimize the sparse matrix-vector multiplication operation, which is the most time consuming part of the kernel polynomial method used in the GFBMC. Also we will plan to develop a quantum molecular dynamics method for electrons coupled to the classical degrees of freedom to simulate non-equilibrium quantum dynamics.

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] "Anisotropic two-dimensional electron gas at the $LaAlO_3/SrTiO_3$ (110) interface", A. Annadi, Q. Zhang, X. Renshaw Wang, N. Tuzla, K. Gopinadhan, W. M. Lü, A. Roy Barman, Z. Q. Liu, A. Srivastava, S. Saha, Y. L. Zhao, S. W. Zeng, S. Dhar, E. Olsson, B. Gu, S. Yunoki, S. Maekawa, H. Hilgenkamp, T. Venkatesan & Ariando, Nature Communications **4**, 1828/1-7 (2013).

[2] "Long-range spin current driven by superconducting phase difference in a Josephson junction with double layer ferromagnets", S. Hikino, and S. Yunoki, Phys. Rev. Lett. **110**, 237003/1-5 (2013).

[3] "Rocksalt SnS and SnSe: Native topological crystalline insulators", Y. Sun, Z. Zhong, T. Shirakawa, C. Franchini, D. Li, Y. Li, and S. Yunoki, and Xing-Qiu Chen, Phys. Rev. B **88**, 235122/1-6 (2013).

[4] "Theoretical study of insulating mechanism in multiorbital Hubbard models with a large spin-orbit coupling: Slater versus Mott scenario inSr_2IrO_4", H. Watanabe, T. Shirakawa, and S. Yunoki, Phys. Rev. B **89**, 165115/1-13 (2014).

[5] "Unexpectedly high pressure for molecular dissociation in liquid hydrogen by electric simulation", G. Mazzola, S. Yunoki, and S. Sorella, Nature Communications **5**, 3487/1-6 (2014).

(2) Conference Papers

[6] "Quantum Monte Carlo study of the half-filled Hubbard model on the honeycomb lattice", Y. Otsuka, S. Yunoki, and S. Sorella, J. Phys.: Conf. Ser. **454**, 012045/1-6 (2013).

[7] "Variational Monte Carlo study for the insulating mechanism of Sr_2IrO_4: from the viewpoint of energy gain", H. Watanabe, T. Shirakawa, and S. Yunoki, J. Phys.: Conf. Ser. **454**, 012047/1-6 (2013).

[8] "A study of parallelizing O(*N*) Green-function-based Monte Carlo method for many fermions coupled with classical degrees of freedom", S. Zhang, S. Yamagiwa, and S. Yunoki, J. Phys.: Conf. Ser. **454**, 012049/1-15 (2013).

[9] "Superfluidity of one-dimensional trapped fermionic optical lattices with spatially alternating interactions", A. Yamamoto and S. Yunoki, J. Phys.: Conf. Ser. **454**, 012067/1-5 (2013).

[10] "Theoretical studies of a three-band Hubbard model with a strong spin-orbit coupling for 5d transition metal oxide Sr_2IrO_4", T. Shirakawa, H. Watanabe, and S. Yunoki, J. Phys.: Conf. Ser. **454**, 012068/1-8 (2013).

[11] "Photoinduced spin-order destructions in one-dimensional extended Hubbard model", H. Lu, S. Sota, H. Matsueda, J. Bonča and T. Tohyama, J. of Phys.: Conf. Ser. **454**, 012079/1-7 (2013).

[12] "A novel superconductivity in Ir oxides with a large spin-orbit coupling", H. Watanabe, T. Shirakawa, and S. Yunoki, J. Kor. Phys. Soc. **62**, 1848-1851 (2013).

[13] "Mott transition in the two-dimensional π-flux phase", Y. Otsuka, S. Yunoki, and S. Sorella, J. Phys. Soc. Jpn. Suppl., 5 pages, in press.

(3) Invited Talks

[14] "Spin liquid phases in strongly correlated lattice models", S. Sorella, 25th Annual Workshop on Recent Developments in Electronic Structure Theory, Williamsburg (USA), June 2013.

[15] "Anisotropic two-dimensional electron gas at the $LaAlO_3/SrTiO_3$ (110) interface", S. Yunoki, 20th Workshop on Oxide Electronics, Singapore, September 2013.

[16] Lectures on "Spin liquid phases in strongly correlated lattice models", S. Sorella, Quantum Spin Liquids: From Theory to Numerical Simulations, Trieste (Italy), September 2013.

[17] "Massively parallel two-dimensional density matrix renormalization group method", S. Sota, CMSI Kobe International Workshop 2013: Recent Progress in Tensor Network Algorithms, Kobe (Japan), October 2013.

[18] "Novel unconventional superconductivity in J_{eff}=1/2 Mott insulator for Ir oxides", S. Yunoki, First-QS^{2}C Workshop on "Emergent Phenomena of Correlated Materials", Tokyo (Japan), November 2013.

[19] "Mott transition in the Hubbard model on the honeycomb lattice", Y. Otsuka, S. Yunoki, and S. Sorella, Condensed Matter Seminar in Tsukuba university, Tsukuba (Japan), November 2013.

[20] "Development of massively parallel density matrix renormalization group method", S. Sota, International Workshop on Massively Parallel Programming Now in Molecular Science, Tokyo, (Japan) February 2014.

(4) Posters and Presentations

[21] "Ground-state phase diagram of the half-filled Hubbard model on the honeycomb lattice", Y. Otsuka, S. Yunoki, and S. Sorella, 3rd AICS International Symposium, Kobe (Japan), February 2013.

[22] "Mott transition in the two-dimensional π-flux phase", Y. Otsuka, S. Yunoki, and S. Sorella, International Conference on Strongly Correlated Electron Systems (SCES2013), Tokyo (Japan), August 2013.

[23] "Density matrix renormalization group study of the half-filled Hubbard model on the triangular lattice", S. Sota, K. Shinjo, T. Tohyama、and S. Yunoki, International Conference on Strongly Correlated Electron Systems (SCES2013), Tokyo (Japan), August 2013.

[24] "Mott transition in the π-flux phase", Y. Otsuka, S. Yunoki, and S. Sorella, JPS 2013 Fall meeting, Tokushima (Japan), September 2013.

[25] "Two-dimensional density matrix renormalization group method on the K-computer II", S. Sota, K. Shinjo, T. Tohyama、and S. Yunoki, 68th JPS annual meeting, 25aKH-3, Hiratsuka (Japan), September 2013.

[26] "Parallelization of kernel polynomial method for magnetic Skyrmion", S. Zhang and S. Yunoki, RIKEN Booth, Supercomputing 13, Denver (USA), November 2013.

Computational Biophysics Research Team

1. Team members

Yuji Sugita (Team Leader)

Osamu Miyashita (Senior Research Scientist)

Jaewoon Jung (Research Scientist)

Chigusa Kobayashi (Research Scientist)

Raimondas Galvelis (Postdoctoral Researcher)

Yasuhiro Matsunaga (RIKEN Special Postdoctoral Researcher)

Naoyuki Miyashita (Research Scientist (Concurrent))*

Tadashi Ando (Research Scientist (Concurrent))*

Yasuhito Karino (Postdoctoral Researcher (Concurrent))*

Yumi Kashihara (Postdoctoral Researcher (Concurrent))*

Takaharu Mori (Research Scientist (Concurrent))**

Takao Yoda (Visiting Scientist) ***

Mitsunori Ikeguchi (Visiting Scientist)****

Hiromi Kano (Assistant (Concurrent))*

* The main affiliation of these people is Laboratory for Biomolecular Function Simulation, Computational Biology Research Core, RIKEN Quantitative Biology Center.

** The main affiliation is RIKEN Theoretical Molecular Science Laboratory.

*** The main affiliation is Nagahama Bio Institute.

**** The main affiliation is Yokohama City University.

2. Research Activities

In molecular biology, atomic structures of proteins and other biomolecules provide essential information for understanding their biomolecular functions. Recently, MD simulations of biomolecules in solution or in biological membrane are often performed to elucidate the relationship between conformational dynamics and biomolecular functions. However, the conventional approaches have, at least, two major difficulties and cannot be compared directly to the experimental data. The first one is that simulation time of all-atom MD simulation is limited to about microsecond and this time scale is much shorter than that of slow conformational dynamics of proteins. The second difficulty is that the cellular environments are hardly involved in the MD simulations due to the size limitation of MD simulation. In this team, we have developed novel high-performance MD software, which we call GENESIS, to perform MD simulations of biomolecules efficiently on K computer. We aim to perform biomolecular simulations under realistic cellular environments as long as possible. The development of new

algorithms and the use of multi-scale and multi-resolution models are effective for large-scale MD simulations. In this team, we develop these methods and models in biomolecular simulations, also.

3. Research Results and Achievements

3.1. New Inverse Lookup Table for the evaluations of nonbonded interactions

We have developed a new lookup table for efficient short-range non-bonded interactions. Major bottleneck in MD is the calculation of non-bonded interactions of van der Waals and electrostatic. With spherical truncation (cutoff approximation) and particle mesh Ewald (PME), calculation order or van der Waals and real space electrostatic is reduced from O(n2) to O(n). However, these interactions are still the main bottleneck of MD, and they include very time-consuming inverse square roots and complementary error functions. To avoid such time-consuming operations while keeping accuracy, we proposed a new lookup table for short-range interaction in PME by defining energy and gradient as a linear function of inverse distance squared. In our lookup table approach, the table density is proportional to the inverse of squared distance. The new table increases accuracy by assigning large number of points at small pair distances where energy/gradients changes rapidly (Figure 1a). Despite of inverse operations in our approach, the new lookup table scheme allows fast evaluation due to small cache misses (Figure 1b). Overall, linear 1/R2 lookup table is highly promising for MD from the point of view of both accuracy and efficiency.

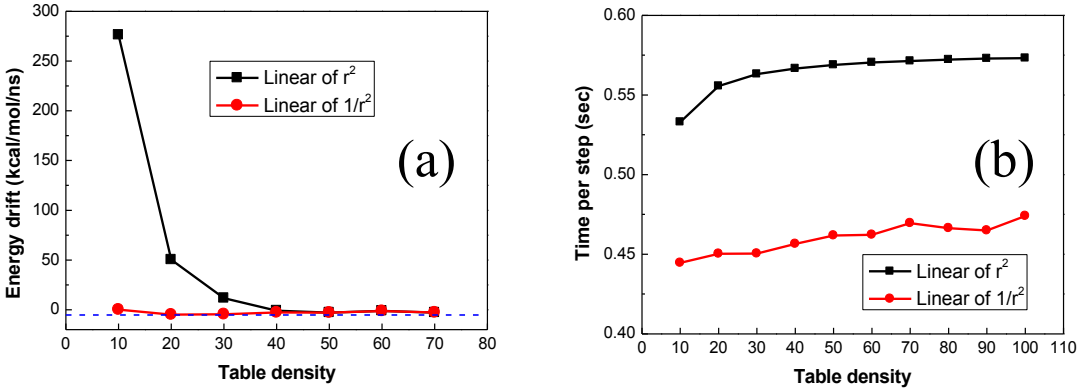


Figure 1. (a) Energy drift value according to the number of table points in unit section. (b) Computational time for one step calculation.

3.2 Midpoint Cell Method for hybrid parallelization

We have developed a new hybrid (MPI+OpenMP) parallelization scheme for molecular dynamics (MD) simulations by combining a cell-wise version of the midpoint method with pair-wise Verlet lists. In this scheme, which we call the midpoint cell method, simulation space is divided into subdomains, each of which is assigned to a MPI processor. Each subdomain is further divided

into small cells. The interaction between two particles existing in different cells is computed in the subdomain containing the midpoint cell of the two cells where the particles reside. In each MPI processor, cell pairs are distributed over OpenMP threads for shared memory parallelization. The midpoint cell method keeps the advantages of the original midpoint method, while filtering out unnecessary calculations of midpoint checking for all the particle pairs by single midpoint cell determination prior to MD simulations. Distributing cell pairs over OpenMP threads allows for more efficient shared memory parallelization compared with distributing atom indices over threads. Furthermore, cell grouping of particle data makes better memory access, reducing the number of cache misses. The parallel performance of the midpoint cell method on the K computer showed scalability up to 512 and 32,768 cores for systems of 20,000 and 1 million atoms, respectively. One MD time step for long-range interactions could be calculated within 4.5 ms even for a 1 million atoms system with PME electrostatics (Figure 2).

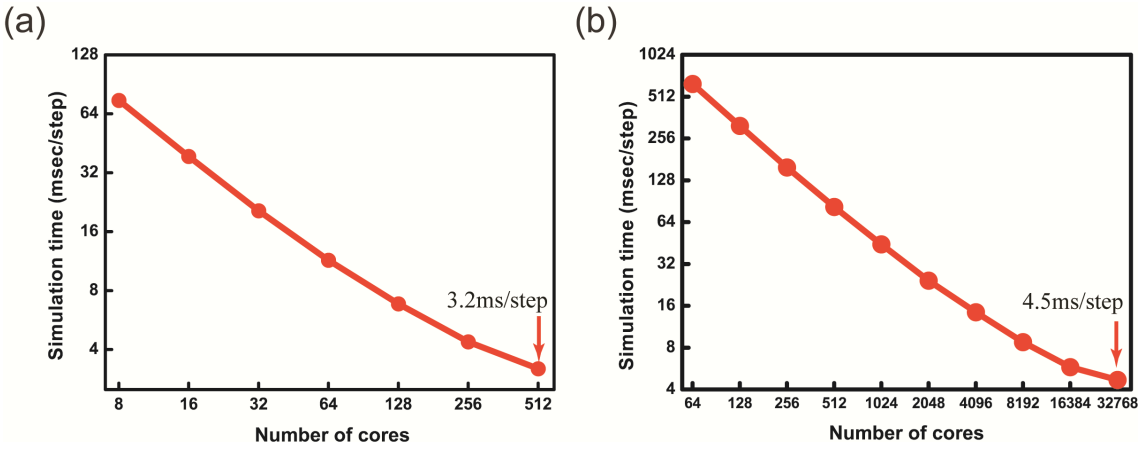


Figure 2. Simulation time (ms/step) for (a) 22,000 and (b) 1 million atoms systems.

3.3 Development of high-performance software GENESIS

GENESIS (Generalized Ensemble Simulation System) is a suite of computer program for carrying out MD for biomolecular systems. While most of MD programs have been parallelized for distributed memory parallelization for small and intermediate size systems (< 1 million atoms), GENESIS is optimized with hybrid parallelization by combining MPI with OpenMP for large-scale simulations. For fast evaluation of MD, we introduced lookup table approach and domain decomposition named midpoint cell method, which are already written in the above sections. In GENESIS, we have two simulators: ATDYN (atomic decomposition dynamics) and SPDYN (spatial decomposition dynamics). The former is easy to be modified for developing new methods due to simple parallelization using atomic decomposition, and enhanced sampling algorithms like replica-exchange molecular dynamics (REMD) is available. In ATDYN, in particular, there are special generalized ensemble algorithms named "surface-tension replica-exchange" developed

in our group. SPDYN was written mainly for efficient parallelization and fast evaluation for large systems. For efficient parallelization, Fast Fourier Transform (FFT) that shows the best parallel performance out of all MD programs is also optimized. SPDYN is optimized for K supercomputer, leading 6 ns/day for 100 million atoms system. This is an impressing result because the performance is almost twice faster than that of NAMD on Blue Gene/Q.

GENESIS has the following features:

1) Coarse-grained as well as explicit all-atom MD is available in ATDYN.
2) Parallel input/output (I/O) is available for very large system for efficient memory usage and fast setup.
3) GENESIS is optimized for K supercomputer, but it is also available on PC-clusters.
4) Everything is written in Fortran 90/95/2003 with dynamics memory allocation.
5) GENESIS is free software licensed under GPL version 2.

3.4 Data assimilation algorithm for analyzing conformational dynamics of biomolecules

We have been developing an algorithm for data-assimilation simulations incorporating single-molecule Förster resonance energy transfer (smFRET) measurements. SmFRET measurement is a powerful technique to investigate dynamic behavior of biomolecules as a function of time. However, the interpretation of smFRET data is sometimes difficult since the information is limited only to the distance-like information between two fluorescence dyes. We have been developing a data-assimilation technique, based on the particle filter, to interpret the smFRET data in terms of coarse-grained protein models. This year, we have formulated a likelihood function for smFRET photon counting data, by modeling the numbers of observed photons from the two dyes as inhomogeneous Poisson processes. We have implemented the likelihood function in GENESIS and tested the performance of the algorithm by using a simulated FRET-like photon counting data on K computer. Using polyproline as a test case, we have confirmed the performance using 131,072 replicas (particles) and 8,192 nodes of K computer.

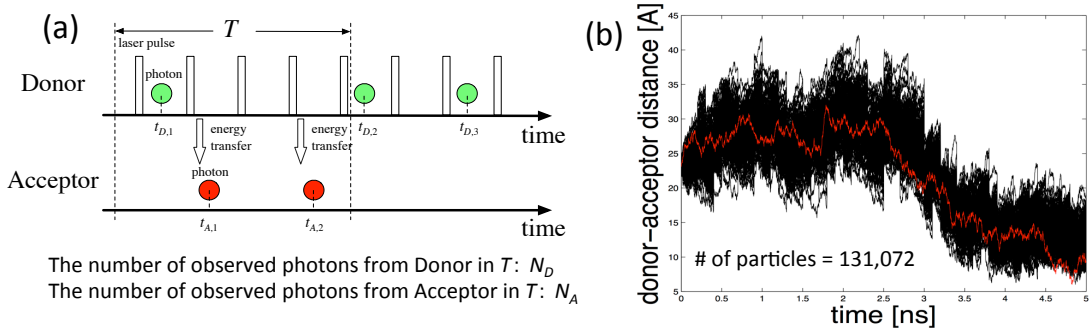


Figure 3. (a) Schematic picture of smFRET photon counting data. (b) Inference for the distance between two fluorescence dyes attached to polyproline from simulated smFRET photon

counting data. The red line indicates the true answer, and black lines are replicas (particles).

3.5 Motion tree algorithm for analysis of large domain motions of proteins

Proteins are known to take their own three-dimensional structures in physiological conditions. The structures are experimentally determined in crystal conditions (with X-ray crystallography) or in solution (with NMR or others). However, in physiological conditions or in cellular environments, proteins don't behave as rigid bodies but show significant flexibility due to thermal noises. Furthermore, some proteins undergo large domain motions in their reaction cycle, utilizing ATP hydrolysis or proton motive forces. Sarco(endo)plasmic reticulum Ca^{2+}-ATPase (SERCA), which transports Ca^{2+} across biological membranes against a large concentration gradient, is one of the best-studied membrane proteins. In classical E1/E2 theory, SERCA takes at least two different physiological states, E1 and E2: in the E1 state, the transmembrane binding sites have high affinities for Ca^{2+}, whereas the affinities are greatly reduced in the E2 state. In addition to the binding and release of Ca^{2+}, ATP hydrolysis and dephosphorylation at the phosphorylation residue, Asp351, introduces more physiological states.

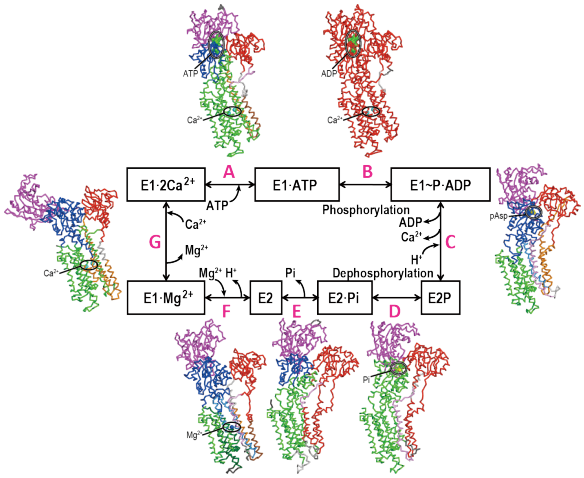


Figure 4. Reaction cycle of SERCA and rigid domains in MTs on reaction steps

To characterize its conformational motions, we illustrate 'Motion Tree (MT)' based on seven crystal structures of SERCA. MT is a tree diagram that represents hierarchical domain-motion. (Koike *et al.*, *J. Mol. Biol.*, 2014) We investigate the relationship between local conformational changes and function of SERCA based on MTs. In addition, we determine 'common rigid domains (CRD)' that keep their structural rigidity during the whole reaction cycle. The analysis allows discussion of how the protein utilizes both structural rigidity and flexibility for pumping Ca^{2+} across the membrane. We also investigate local conformational changes upon a dissociation of Pi and Mg^{2+} from the nucleotide-binding site using atomistic molecular dynamics (MD) simulations. The simulations reinforce the notion of a conformational change upon binding/dissociation of the ligands. We emphasize that MT detects such motions automatically without extensive biological knowledge, suggesting general applicability to domain movements in other membrane proteins to deepen the understanding of protein structure and function.

3.6 Development of new meta-dynamics algorithms

The understanding of biological systems by atomistic-level simulations requires free energy calculations, which inherently is a problem of conformation space sampling. Metadynamics, an adaptive-biasing technique, has proven its efficiency to accelerate sampling. The method estimates the free energy by iteratively updating a biasing potential in a predefined collective variable space. In particular, we were focused on the multi-replica algorithms of metadynamics, which could be efficiently implemented on the massively parallel computers (such as K computer). Currently ATDYN supports several mutil-replica algorithms: multiply-walker, parallel-tempered, and bias-exchange. We have demonstrated the advantages of metadynamics to enhance and parallelize sampling effort with several systems, including alanine pentapeptide (Figure 5). Finally, novel replica-exchange schemes are being investigated to increase efficiency of the multi-replica metadynamics by optimizing exchange rates and patterns. Additionally, this allows a larger number of collective variables to be used, enabling the efficient simulations of more complex systems and phenomena.

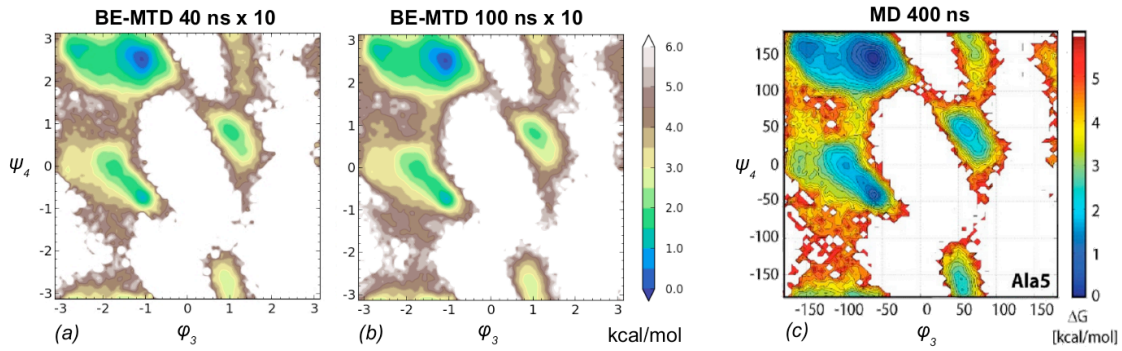


Figure 5. Free energy surface along two backbone dihedral angles (φ_3, ψ_4) of alanine pentapeptide (Ala5) obtained from (a) 40 ns and (b) 100 ns of 10-replica bias-exchange metadynamics (BE-MTD) simulations, and, for comparison, from (c) 400 ns of an MD simulation (adapted from R.B. Best, et al., *J. Chem. Theory Comput.*, 2012, 8(9): 3257–3273).

3.7 Computational analysis of low-resolution structural data from XFEL and EM

We have been developing algorithms to construct atomistic models from low-resolution structural data. Cryo-EM and newly emerging XFEL experiments provides new structural information that are not available in traditional X-ray crystallography, since these experiments can be performed without the crystallization of target systems. However, on the other hand, the data from Cryo-EM and XFEL are at low-resolution without atomic details, and thus need to be complimented by other information to construct atomic models. We have been implementing the algorithms in GENESIS to perform flexible fitting of atomic structures into such low-resolution data. Using generalized ensemble algorithms embedded in GENESIS, the accuracy and efficiency of fittings can be enhanced.

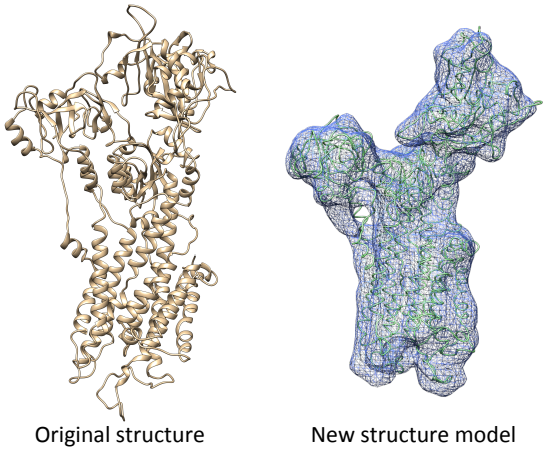


Figure 6. A result of flexible fitting using GENESIS. The original structure (left) is deformed using molecular dynamics simulation to fit the low-resolution data.

4. Schedule and Future Plan

We have released the first version of GENESIS program as free software under GPL license v2. We continue to develop the software for improving its performance in MD simulations and adding new functions and molecular models. To show the performance and reliability of GENESIS on K computer, we will perform simulations of large biomolecules like Ribosomes, membrane proteins, and so on.

We have already implemented the efficient evaluations of non-bonded interactions and their forces. Another time consuming part is non-bonded reciprocal interactions in particle mesh ewald (PME) approximation. In PME, the reciprocal interaction is evaluated using FFT (Fast Fourier Transform) computation, which usually show poor parallel scalability. We plan to improve the performance of FFT on parallel computers.

Multi-scale and multi-resolution models are important to simulate large-scale conformational changes of membrane proteins or protein complexes under cellular environment. In GENESIS, we will introduce these models for efficient conformational sampling of large biomolecular systems. We also plan to implement QM/MM hybrid simulations on GENESIS for simulating enzyme reactions.

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] Jaewoon Jung, Takaharu Mori, and Yuji Sugita: "Midpoint Cell Method for Hybrid (MPI+OpenMP)

Parallelization of Molecular Dynamics Simulations", J. Comput. Chem., in press.

[2] L.S. Ahlstrom, and Osamu Miyashita: "Packing interface energetics in different crystal forms of the λ Cro dimer", Proteins, in press.

[3] Takaharu Mori, Jaewoon Jung, and Yuji Sugita: "Surface-tension replica-exchange molecular dynamics method for enhanced sampling of biological membrane systems", J. Chem. Theory Comput. **9** (2013) 5629-5640.

[4] Jaewoon Jung, Takaharu Mori, and Yuji Sugita: "Efficient lookup table using a linear function of inverse distance squared", J. Comput. Chem. **34** (2013) 2412-2420.

[5] Logan S. Ahlstrom, Joseph Lee Baker, Kent Ehrlich, Zachary T. Campbell, Sunita Patel, Ivan I. Vorontsov, Florence Tama, Osamu Miyashita: "Network visualization of conformational sampling during molecular dynamics simulation", J. Mol. Graph Model. **46** (2013) 140-149.

[6] Yasuhiro Matsunaga, Akinori Baba, Chun-Biu Li, John E. Straub, Mikito Toda, Tamiki Komatsuzaki, and R. Stephen Berry: "Spatio-temporal hierarchy in the dynamics of a minimalist protein model", J. Chem. Phys. **139** (2013) 215101.

(2) Invited Talks

[7] Yasuhiro Matsunaga: "Finding Conformational Transition Pathways in Biomolecules with the String Method and Sequential Data Assimilation", Rare Event Sampling and Related Topics I, ISM, Tokyo, Japan, March 4-5, 2014.

[8] Jaewoon Jung: "Development of GENESIS for large scale molecular dynamics simulation", Bio-Supercomputing Winter school, Atagawa, January 23-24, 2014.

[9] Osamu Miyashita, Atsushi Tokuhisa, Florence Tama: "An Overview of Single Biomolecular Imaging by X-ray Free Electron Laser", Institut de Minéralogie et de Physique des Milieux Condensés, France, December 16, 2013.

[10] Jaewoon Jung: "Development of GENESIS for large scale molecular dynamics simulation", Workshop on Molecular Simulations of Biophysics and Biochemistry, Kobe, November 21, 2013.

[11] Yasuhiro Matsunaga: "Sequential data assimilation of single-molecule FRET photon-counting data by using molecular dynamics simulations", Workshop on Molecular Simulations of Biophysics and Biochemistry, Kobe, November 21, 2013.

[12] Yuji Sugita, Ryuhei Harada, Isseki Yu, Takaharu Mori, Jaewoon Jung, and Michael Feig: "Biomolecular Simulations under Cellular Crowding Environment", ICMS 2013, Kobe, November 18-20, 2013.

[13] Jaewoon Jung, "Development of GENESIS for large scale molecular dynamics simulation", CMSI International Satellite Meeting 2013 in Nagoya, Nagoya, October 17-19, 2013.

[14] Yuji Sugita: "Replica-Exchange Molecular Dynamics Simulations of Membrane Protein Systems", The Snowmass Biophysics Workshop on Free-Energy Calculations, Snowmass,

Colorado, USA, July 15-19, 2013.

[15] Yuji Sugita: "Molecular Dynamics Simulations of MATE multi-drug transporter", The Snowmass Biophysics Workshop on Membrane and Membrane Proteins, Snowmass, Colorado, USA, July 22-26, 2013.

[16] Osamu Miyashita: "Effect of Crystal Packing on Protein Conformation and Dynamics", Nagoya University, Nagoya, May 27, 2013.

[17] Yuji Sugita and Takaharu Mori: "Surface Area in Protein-Membrane Simulation Systems, Biophysical Society Meeting on Membrane Protein Folding", Seoul, South Korea, May 19-22, 2013.

(3) Posters and Presentations

[18] Chigusa Kobayashi and Yuji Sugita: "Conformational change of SERCA upon alternating protonation states in Ca^{2+}-binding site", The 4th AICS International Symposium, Kobe, December 2-3, 2013.

[19] Jaewoon Jung, Takaharu Mori, and Yuji Sugita, "Midpoint cell method for hybrid (MPI+OPENMP) parallelization of Molecular Dynamics", The 4th AICS International Symposium, Kobe, December 2-3, 2013.

[20] Jaewoon Jung, Takaharu Mori, and Yuji Sugita: "Midpoint cell method for hybrid (MPI+OPENMP) parallelization of Molecular Dynamics", ICMS 2013, Kobe, November 18-20, 2013.

[21] Isseki Yu, Takaharu Mori, Jaewoon Jung, Ryuhei Harada, Yuji Sugita, and Michael Feig: "All-atom Modelling and Molecular Dynamics Simulation of the Cytoplasm of Mycoplasma Genetalium", ICMS 2013, Kobe, November 18-20, 2013.

[22] Chigusa Kobayashi and Yuji Sugita: "Conformational change of SERCA upon alternating protonation states in Ca^{2+}-binding site", ICMS 2013, Kobe, November 18-20, 2013.

[23] Chigusa Kobayashi and Yuji Sugita: "Conformational change of SERCA upon alternating protonation states in Ca^{2+}-binding site", ICMS 2013, Kobe, November 18-20, 2013.

[24] Yasuhiro Matsunaga, Takaharu Mori, Jaewoon Jung, and Yuji Sugita: "Sequential data assimilation of single-molecule FRET photon-counting data by using molecular dynamics simulations", Workshop on Modeling Biomolecular Systems in Cellular Environments, Kyoto, October 31 - November 1, 2013.

[25] Raimondas Galvelis and Yuji Sugita: "Metadynamics: Implementation in GENESIS and Demonstration of Efficient Simulations", Workshop on Modeling Biomolecular Systems in Cellular Environments, Kyoto, October 31 - November 1, 2013.

[26] Yasuhiro Matsunaga, Takaharu Mori, Jaewoon Jung, and Yuji Sugita: "Sequential data assimilation of single-molecule FRET photon-counting data by using molecular dynamics simulations", Workshop on Modeling Biomolecular Systems in Cellular Environments, Kyoto,

October 31 - November 1, 2013.

[27] Jaewoon Jung, Takaharu Mori, and Yuji Sugita: "Efficient Lookup Table using a Linear Function of Inverse Distance Squared", The 51th Annual Meeting of the Biophysical Society of Japan, Kyoto, October 28–30, 2013.

[28] Isseki Yu, Takaharu Mori, Jaewoon Jung, Ryuhei Harada, Yuji Sugita, and Michael Feig: "All-Atom Molecular Dynamics Simulation of Bacterial Cytoplasm", The 51th Annual Meeting of the Biophysical Society of Japan, Kyoto, October 28–30, 2013.

[29] Takaharu Mori, Jaewoon Jung, and Yuji Sugita: "Acceleration of lipid lateral diffusion by generalized-ensemble molecular dynamics simulation", The 51th Annual Meeting of the Biophysical Society of Japan, Kyoto, October 28–30, 2013.

[30] Chigusa Kobayashi and Yuji Sugita: "Conformational change of SERCA upon alternating protonation states in Ca^{2+}-binding site", The 51th Annual Meeting of the Biophysical Society of Japan, Kyoto, October 28–30, 2013.

[31] Raimondas Galvelis and Yuji Sugita: "Metadynamics: Implementation in GENESIS and Demonstration of Efficient Simulations", The 51th Annual Meeting of the Biophysical Society of Japan, Kyoto, October 28–30, 2013.

[32] Yasuhiro Matsunaga, Takaharu Mori, Jaewoon Jung, and Yuji Sugita: "Sequential data assimilation of single-molecule FRET photon-counting data by using molecular dynamics simulations", The 51th Annual Meeting of the Biophysical Society of Japan, Kyoto, October 28–30, 2013.

[33] 小林千草、小池亮太郎、太田元規、杉田有治: "Motion Tree 法を用いた SERCA のリガンド解離における構造変化の解析", 第 13 回日本蛋白質科学会年会, 鳥取、2013 年 6 月 12 日.

[34] Chigusa Kobayashi, Ryotaro Koike, Motonori Ota, and Yuji Sugita: "Conformational changes of SERCA upon dissociation of ligand analyzed with Motion Tree method", Membrane protein folding meeting, Korea, May 20, 2013.

(4) Patents and Deliverables

[35] Generalized-Ensemble Simulation System (GENESIS) is released. 2014/03.
https://aics.riken.jp/labs/cbrt/
http://www.riken.jp/TMS2012/cbp/en/research/software/genesis/index.html

Particle Simulator Research Team

1. Team members

Junichiro Makino (Team Leader)
Keigo Nitadori (Research Scientist)
Masaki Iwasawa (Postdoctoral Researcher)
Ataru Tanikawa (Postdoctoral Researcher)
Miyuki Tsubouchi (Technical Staff)

2. Research Activities

We are developing particle-based simulation software that can be used to solve problems of vastly different scales.

Simulation schemes for hydrodynamics and structural analysis can bedivided into grid-based and particle-based methods (see Figure 1). In grid-based methods, the computational region is mapped to regular or irregular grids. Continuous distributions of physical values are represented by discrete values at grid points, and the governing partial differential equation is approximated to a set of finite difference equations.

In the case of the particle-based methods, physical values are assigned to particles, while the partial differential equation is approximated by the interactions between particles.

Both methods are widely used, and they have their advantages and disadvantages. The computational cost of grid-based schemes is generally lower than that of particle-based methods with similar number of freedoms. Thus, if an near-uniform grid structure is appropriate for the problem to be solved, grid-based methods perform better.

The advantage of the particle-based methods comes from the fact that they use "Lagrangian" schemes, in which the particles move following the motion of the fluid in the case of the CFD calculation. In the case of grid-based methods, we generally use "Eulerian" schemes, in which the grid points do not move.

There are three points in which the Lagrangian schemes are better than Eulerian schemes.

One is that the Lagrangian schemes are, to some extent, adaptive to the requirement of the accuracy, since when a low-density region is compressed to become high density.

Second one is that the timestep criteria are quite different. In the case of the Lagrangian schemes, the timestep is determined basically by local sound velocity, while in the Eulerian scheme by global velocity. Thus, if a relatively cold fluid is moving very fast, the timestep for the Eulerian schemes can be many orders of magnitude shorter than that for Lagrangian schemes.

Finally, in the case of fast-moving low-temperature fluid, the required accuracy would be very high for Eulerian scheme, since the error comes from the high velocity, while that error would be transferred to internal energy of the fluid element which is much smaller than that of the kinetic motion.

Of course, there are disadvantages of Lagrangian schemes. The primary one is the difficulty of construction of such schemes in two or higher dimensions. In the case of one-dimensional calculation, it is easy to move grid points following the motion of the fluid, but in two or higher dimensions, the grid structure would severely deform if we let the grid points follow the flow. Thus, we have to reconstruct the grid structure every so often. This requirement causes the program to become complex. Moreover, reconstruction of the grid structure (so called remeshing) means we lose numerical accuracy.

Particle-based methods "solve" this difficulty by not requiring any mesh. In particle-based methods, particles interact with its neighboring particles, not through some connection through grid, but through distance-dependent kernel functions. Thus, there is no need of remeshing. As a result, particle-based schemes are simple to implement, and can give reasonable results even when the deformation is very large. Another important advantage is that it is relatively easy to achieve high efficiency with large-scale particle-based simulation.

In the case of grid-based schemes, in order achieve some adaptivity to the solution, we have to use either irregular grid or regular grid with adaptive mesh refinment. In both cases, adaptivity breaks the regularity of the mesh structure, resulting in non-contiguous access to the main memory. In the case of the particle-based schemes, it does require some irregular memory access, but it is relatively straightforward to make good use of spacial locality, and thereby achieving high efficiency. Similarly, very high parallel performance can be achieved.

However, it has its own problems. In the case of the SPH method, it has been known that the standard scheme cannot handle the contact discontinuity well. It also require rather strong artificial viscosity, which results in very low effective Reynolds number.

Thus, in many fields of computational sciences, many groups are working on implementation of high-performance particle-based simulation codes for their specific problem.

One serious problem here is that, high-performance, highly-parallel simulation codes for particle-based simulations are becoming more and more complex, in order to make full use of modern supercomputers. We need to distribute particles to many computing nodes in an appropriate way, so that the communication between nodes is minimized and at the same time near-optimal load balance is achieved. Within each nodes, we need to write an efficient code to find neighbor particles, rearrange data structure so that we can make good use of the locality, make good use of multiple cores and SIMD units within each core.

Even for the case of very simple particle-particle interaction such as the Lenard-Jones potential or Coulomb potential, the calculation code tends to be very large, and since the large fraction of the code is written to achieve a high efficiency on a specific architecture, it becomes very hard to port a code which is highly optimized to one architecture to another architecture.

Our goal is to develop a "universal" software that can be applied to a variety of problems whose scales are vastly different. In designing such universal software, it is important to ensure that it runs efficiently on highly parallel computers such as the K computer. Achieving a good load balance with particle-based simulation is a difficult task, since using a regular spatial decomposition method causes severe load imbalance, though this works well for grid-based software. Consequently, we have developed an adaptive decomposition method that is designed to work in a way that the calculation time on each node is almost the same, resulting in near-optimal load balance. The strategy to develop such a universal software is as follows.

We first construct a highly parallel and very efficient implementation of the TreePM algorithm for gravitational N-body problem. This is actually not a completely new implementation, but the GreeM code developed by researchers of the Strategic Program for Innovative Research (SPIRE) Field 5 “The origin of matter and the universe. In collaboration with the Field 5 researchers, we improve the efficiency of the code and study the issues of the data structure, domain decomposition, load balance strategy etc.

In the second stage, we will develop a prototype of the parallel particle simulation platform. We will design the platform so that it can be used for multiple physical systems. In practice, we consider the following three applications as the initial targets.

1. Gravitational N-body simulation
2. Smoothed Particle Hydrodynamics
3. Molecular Dynamics

In the meantime, we will also investigate the way to improve the performance and accuracy of the current particle-based algorithms for hydrodynamics.

3. Research Results and Achievements

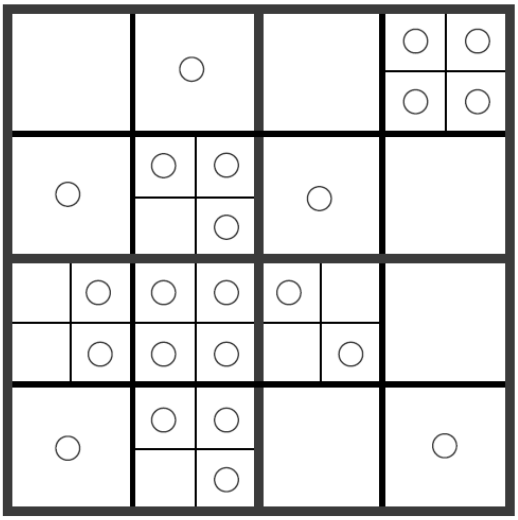
As we stated in section 2, we are working on the three major subtopics, in order to develop the universal platform for particle simulations.

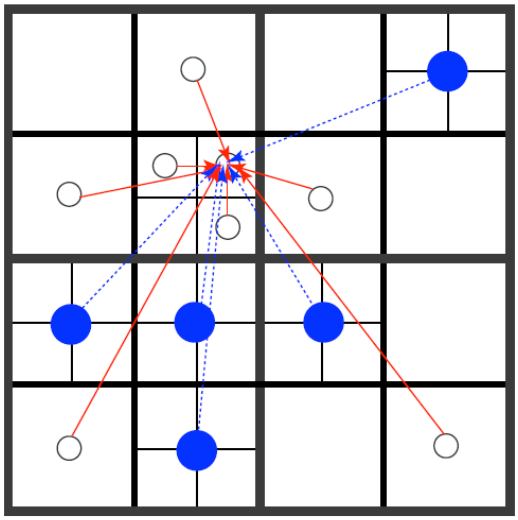
In the following, we briefly describe the status of our research in each subtopic.

3.1. High-performance gravitational N-body solver

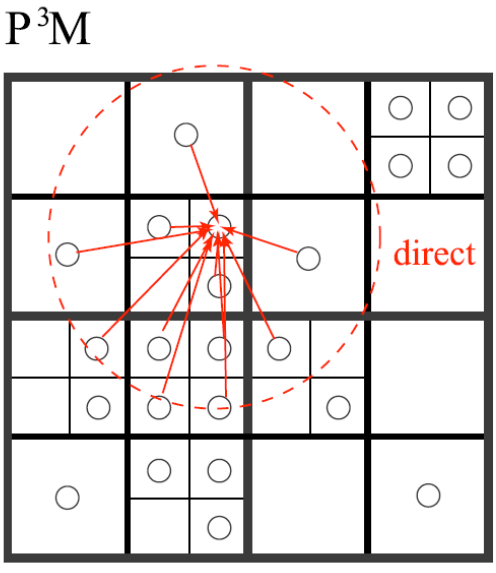
In collaboration with the researchers of researchers of the Strategic Program for Innovative Research (SPIRE) Field 5 "The origin of matter and the universe, we have developed an extremely high performance gravitational N-body solver, GreeM, for the K computer. It achieved, as of November 2012, the sustained performance of 5.67 petaflops (55% of the theoretical peak performance of the K computer). Even more important is its performance measured in the unit of the number of particles updated per second. GreeM on K integrates 4 x 10^{11} particles per second. Researchers in the US developed a similar calculation code on the BG/Q, and its measured speed was 1.6 x 10^{11} particles per second, on the BG/Q machine with the peak speed of 20Pflops. Thus GreeM on K is about 2.4 times faster than the best competing code on a machine nearly two times faster than the K computer. In other words, GreeM on K is about five times more efficient than the best competing code. The numerical accuracy was similar. In the following, we briefly describe the method used and the possible reason for the performance difference between GreeM on K and the calculation on BG/Q. The full detail of the GreeM code is discussed in Ishiyama et al (2012).

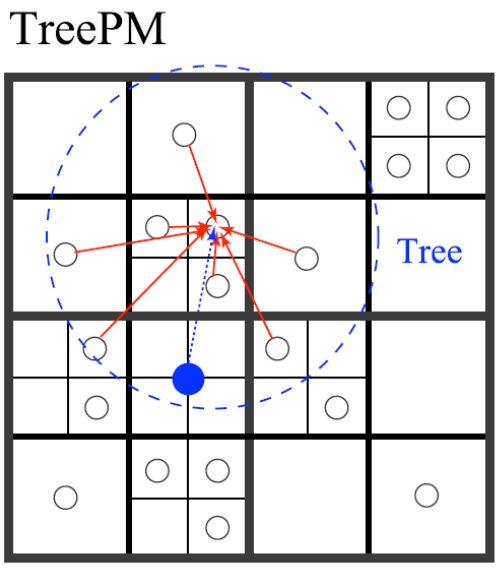
We use the TreePM algorithm as the basic method for the evaluation of gravitational interaction between particles. TreePM is a combination of the tree method and the P^3M (particle-particle particle-mesh) scheme. Figure 1 shows the basic idea of the tree algorithm. The space is divided into a hierarchical octree structure (quadtree in the figure). Division is stopped when a cell contains one or no particle. When we calculate the force on a particle, we evaluate the force from a group of particles, with size larger for more distant particles. In this way, we can reduce the calculation cost from $O(N^2)$ to $O(N \log N)$.





The tree algorithm is widely used, but when the periodic boundary condition is applied, we can actually use a more efficient scheme, since we can calculate the long-range, periodic term using FFT. The P^3M scheme has been used for such problem, but it has the serious problem that when the density contrast becomes high, the calculation cost increases very quickly. The TreePM scheme solves this difficulty by using the tree algorithm to evaluate the forces from nearby particles. Even when there are very large number of neighbor particles, the calculation cost does not increase much, since the calculation cost of the neighbor force is proportional to the logarithm of the number of neighbors.

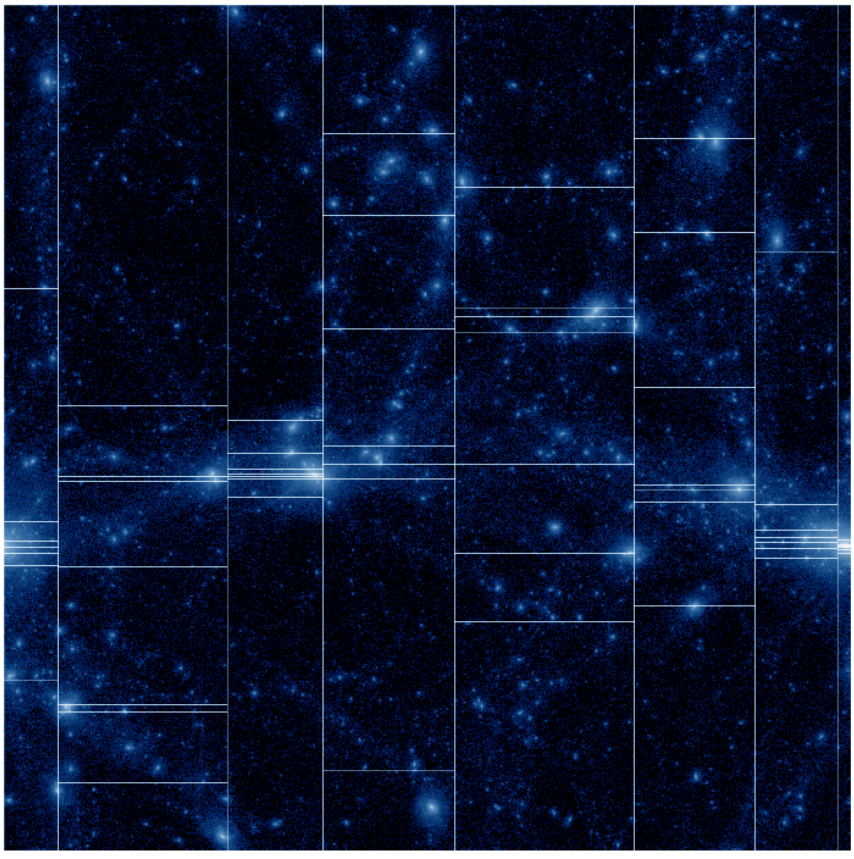




In order to map the problem to the distributed-memory parallel computer such as the K computer, we adopted the approach to divide the space into domains and assign particles in one domain to one calculation node. We used the orthogonal recursive multisection method developed by the team leader some years ago. It is the generalization of the orthogonal recursive bisection (ORB), which has been widely used in many parallel implementations of the tree algorithm.

With ORB, we recursively divide space into two halves, each with the same number of particles. An obvious disadvantage of the ORB approach is that it can utilize the computing nodes of integral powers of two. Thus, in the worst case we can use only half of the available nodes.

The difference between the multisection method and the ORB is that with the multisection method we allow the divisions to arbitrary number of domains, instead of bisection. This would allow too many possible divisions. In our current implementation, we limit the number of levels to three, and make the numbers of divisions at all levels as close as possible. Thus, our domain decomposition is topologically a simple three-dimension grid. This fact makes the multisection method well suited to the machines with the 3D torus network like the K computer.



Originally, with the ORB method the domains contain the same number of particles. It was soon realized that this division did not provide the best load balancing, and people started to use the number of interaction calculations as the measure for the calculation cost. We found that even that is not ideal, and have adopted a much better approach. We simply measure the cost in terms of the CPU seconds, and assign particles the average CPU time. Then we divide the space so that each node should require the same CPU time. This approach turned out to be able to achieve the near-ideal load balance.

Finally, in order to achieve the high efficiency, the efficiency of the force calculation kernel is extremely important. In the case of the K computer, we need to make use of the two-way SIMD unit, and the fact that two units are there. In order to achieve this goal, we developed a new expression for the spline kernel for the force cutoff, which requires only one masked operation. For the force kernel, we have achieved the performance of 72.8% of the theoretical peak or actually 97% of the theoretical limit when we take into account the fact not all floating-point operations are mapped to FMA operations.

Our current implementation is fairly straightforward, and there is nothing unusual. Thus, we have some difficulty in understanding why the competing code is much slower. The most likely reason is that the competing code is the modification of the P^3M code developed by the same group for the Roadrunner supercomputer, which has the IBM Cell processor. Either their code is not yet optimized for the BG/Q, or the original structure of the P^M code resulted in some intrinsic limitation of the performance.

We have developed a "reference code" for gravitational N-body simulation on the K computer. This code is fairly well optimized for the K computer, and shows quite good scalability for even for relatively small-size problems. The asymptotic speed per timestep for large number of nodes is around 7ms. This speed is comparable to that of highly optimized molecular dynamics codes on K, even though our code is designed to handle highly inhomogeneous systems.

We will use this code as the reference implementation for more generalized particle simulation platform which will be described in the next subsection.

3.2. Particle Simulation Platform

We have made detailed specification of the particle simulation platform, which we call FDPS (Framework for Developing Particle Simulator).

The basic idea of FDPS is that the application developer (or the user) specified the way the

particles interact with each other, and the rest is taken care by FDPS. Here, "the rest" includes I/O, domain decomposition and re-distribution of particles, evaluation of interactions between particles, including those in different domains (different MPI processes, for example).

In practice, there are many additional details the user should give. Consider a relatively simple case of particles interacting with soften $1/r$ potential. There are a number of small but important points one has to decide on. For example, what algorithm should be used for the interaction calculation? Even if we limit the possibilities to reasonably adaptive schemes for open boundary problems, we have the choice between Barnes-Hut tree and FMM. For both algorithms, there are many different ways to parallelize them on distributed-memory parallel computers. Also, there are infinitely many variations for the time integration schemes.

The base layer of FDPS offers the domain decomposition based on the recursive multisection algorithm (Makino 2004), with arbitrary weighting function for the load balancing (Ishiyama et al 2009). It also offers the parallel implementation of interaction calculation between particles.

The domain decomposition part takes the array of particles on each node as the main argument. It then generates an appropriate domain for each node, redistribute particles according to their locations, and returns.

The interaction calculation part takes the array of particles, the domain decomposition structure, and the specification of the interaction between particles as main arguments. The actual implementation of this part need to take into account a number of details. For example, the interaction can be of long-range nature, such as gravity, Coulomb force, and interaction between computational elements in the boundary element method (BEM). In this case, the user should also provide the way to construct approximations such as the multiple expansion and the way to estimate error. The interaction might be of short-range nature, with either particle-dependent or independent cutoff length. In these cases, the interaction calculation part should be reasonably efficient in finding neighbor particles.

We have completed the specification document for API of these part, and currently working on the prototype (single-node) implementation of this API.

3.3. Improvements on SPH

SPH (Smoothed Particle Hydrodynamics) has been used in many field, including astrophysics, mechanical engineering and civil engineering. Recently, however, it was pointed out that the standard formulation of SPH has numerical difficulty at the contact discontinuity.

We have been working on the possible solution on this problem, and have made two significant steps in this year. The first one is the generalization of the density-independent SPH to an arbitrary equation of state, and the second one is its further generalization which requires the continuity of neither density nor pressure.

The density-independent SPH is a new formulation of SPH we proposed in 2011. It uses the pressure, instead of the density, as the basic variable using which we evaluate the gradient of other quantities. With hydrodynamics, the pressure is continuous everywhere, except at the shock front. In the case of SPH, we use the artificial viscosity so that the physical variables are all continuous and differentiable even at the shock front. Thus, by using pressure as the basic variable, we can avoid the numerical difficulty associated with the contact discontinuity.

In the case of an ideal gas, we can calculate the pressure easily from the internal energy of particles, but if the equation of state is non-ideal, we cannot calculate the pressure explicitly. We can obtain the pressure by solving an implicit equation, and found that the additional cost of solving the equation is actually small. The reason is that we can also integrate the time evolution of the pressure, and therefore can obtain very good initial guess. Iteration with simple direct substitution is stable and fast enough.

We also developed a very different way to achieve the density independence. In DISPH, we used the pressure-energy pair of intensive and extensive thermodynamic variables to construct the volume estimator of a particle. This estimator works great at the contact discontinuity, at which the pressure is almost constant but the density is discontinuous. However, it behaves poorly where the pressure changes rapidly. One example is the surface of a fluid, either that of liquid or self-gravitating gas. Since the pressure at the surface is by definition zero, the volume estimator based on the pressure cannot give a valid volume element.

We constructed an SPH scheme which uses artificial density-like quantity as the base of the volume estimator. It evolves through usual continuity equation, but with additional diffusion term. Thus, we can guarantee the continuity and differentiability of this quantity, except at the initial condition or at the moment when two fluid elements contact with each other. This scheme seems to work extremely well, and we are currently working on the way to extend this scheme so that it can handle free surface accurately.

4. Schedule and Future Plan

We plan to release the first prototype of the platform by FY 2014. It will have the basic abilities to run on large-scale parallel computers with reasonable load-balancing, for multiple forms of the interparticle interaction formula. We will extend this to fully user-specifiable interface to interparticle interactions in the future release.

References

Ishiyama, T. Nitadori, K, and Makino, J., 2012, 4.45 Pflops astrophysical N-body simulation on K computer: the gravitational trillion-body problem, SC '12 Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis Article No. 5 IEEE Computer Society Press Los Alamitos, CA, USA ©2012 ISBN: 978-1-4673-0804-5

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] "Few-body modes of binary formation in core collapse", Tanikawa, Ataru; Heggie, Douglas C.; Hut, Piet; Makino, Junichiro, Astronomy and Computing, Volume 3, p. 35-49.

[2] "The Cosmogrid Simulation: Statistical Properties of Small Dark Matter Halos", Ishiyama, Tomoaki; Rieder, Steven; Makino, Junichiro; Portegies Zwart, Simon; Groen, Derek; Nitadori, Keigo; de Laat, Cees; McMillan, Stephen; Hiraki, Kei; Harfst, Stefan, The Astrophysical Journal, Volume 767, Issue 2, article id. 146, p. 14, (2013).

[3] "Phantom-GRAPE: Numerical software library to accelerate collisionless N-body simulation with SIMD instruction set on x86 architecture", Tanikawa, Ataru; Yoshikawa, Kohji; Nitadori, Keigo; Okamoto, Takashi, New Astronomy, Volume 19, pp. 74-88.

[4] "Merger criteria of multiple massive black holes and the impact on the host galaxy", Tanikawa, A.; Umemura, M. Monthly Notices of the Royal Astronomical Society, Volume 440, Issue 1, pp.652-662.

[5] "Flaring up of the compact cloud G2 during the close encounter with Sgr A*", Saitoh, Takayuki R.; Makino, Junichiro; Asaki, Yoshiharu; Baba, Junichi; Komugi, Shinya; Miyoshi, Makoto; Nagao, Tohru; Takahashi, Masaaki; Takeda, Takaaki; Tsuboi, Masato; Wakamatsu, Ken-ichi, Publications of the Astronomical Society of Japan, Volume 66, Issue 1, id.1.

[6] "Evolution of star clusters in a cosmological tidal field", Rieder, Steven; Ishiyama, Tomoaki; Langelaan, Paul; Makino, Junichiro; McMillan, Stephen L. W.; Portegies Zwart, Simon, Monthly Notices of the Royal Astronomical Society, Volume 436, Issue 4, pp.3695-3706.

[7] "Density-Independent Smoothed Particle Hydrodynamics for a Non-Ideal Equation of State", Hosono, Natsuki; Saitoh, Takayuki R.; Makino, Junichiro, Publications of the Astronomical Society of Japan, Vol.65, No.5, Article No.108, p.11.

[8] "Dynamical evolution of stellar mass black holes in dense stellar clusters: estimate for

merger rate of binary black holes originating from globular clusters", Tanikawa, A., Monthly Notices of the Royal Astronomical Society, Volume 435, Issue 2, pp.1358-1375.

[9] "A Density-independent Formulation of Smoothed Particle Hydrodynamics", Saitoh, Takayuki R.; Makino, Junichiro, The Astrophysical Journal, Volume 768, Issue 1, article id. 44, p. 24, (2013).

(2) Invited Talks

[10] "ポスト「京」プロジェクトハードウェア概要", 牧野　淳一郎、理研和光一AICS 合同シンポジウム「京、ポスト京と基礎物理」2014/1/7。

[11] "理論家からみた統計誤差と系統誤差" 牧野　淳一郎、銀河系目標ミニワークショップ@三鷹 2013/12/27。

[12]「重力相互作用カーネルのチューニング —組み込み関数を用いた手動 SIMD 化」似鳥啓吾、「京」における高速化ワークショップ（高度情報科学技術研究機構（RIST）主催）2013/12/18。

[13] "PC クラスタの終わりの始まり？---エクサ時代のミッドレンジのあり方:" 牧野　淳一郎、PC クラスタシンポジウム 2013/12/12。

[14] "次世代高性能計算機への昨今動き(富田さんの代理的なにか)+ 今後の計算機と計算科学---なぜ我々は 7 年前の間違いを繰り返{す、した}のか" 牧野　淳一郎、計算惑星科学シンポジウム@石垣島 2013/11/23。

[15]「Xeon Phi 上での N 体計算コードの実装」 似鳥　啓吾、東京大学コンピュータ科学専攻講演会、2013/10/9。

[16] "Exascale computers? / Can we believe SPH simulations of Giant Impact?", Jun Makino, Science as Method and Methodology for Problems on the Earth and Life, Sep 15-17, 2013, Nagoya, Japan。

[17] "エクサスケールシステムに向けて --- 分散メモリ超並列アーキテクチャの復活" 牧野淳一郎、第 5 回アクセラレーション技術発表討論会(第 2 種研究会) 2013/9/6。

[18] "Exascale computers in --- 2019?", Jun Makino, Large-Scale simulation of Formation and Evolution of Planetary Systems: Kobe 2013 Summer Workshop, Aug 7-8, 2013, Kobe, Japan.

[19] "京の威力で「見えない宇宙」の正体に迫る —ダークマターの超大規模シミュレーション" 牧野　淳一郎、京コンピュータ・シンポジウム 2013/5/13。

(3) Posters and Presentations

[20] "球状星団におけるコンパクト連星形成", 谷川衝, 2013 年 12 月 25-27 日, 東京大学, 第 26 回理論懇シンポジウム。

[21] "球状星団におけるコンパクト連星形成について", 谷川　衝, 2013 年 11 月 5-6 日, 筑波大学, 第 5 回「学際計算科学による新たな知の発見・統合・創出」シンポジウム —T2K-Tsukuba、HA-PACS による計算科学の発展と、次世代コンピューティングの展望—。

[22] “二重白色矮星の合体時に発生するホットスポットの構造”, 谷川　衝, 2013 年 9 月 10-12 日, 東北大学, 日本天文学会。

[23] “Detection rate of binary black holes formed in globular clusters”, Tanikawa, A., 3-7 Jun 2013, Yukawa Institute for Theoretical Physics Kyoto University, Yukawa International Seminar 2013 Gravitational Waves Revolution in Astronomy & Astrophysics.

Computational Climate Science Research Team

1. Team members

Hirofumi Tomita (Team Leader)
Shin-ichi Iga (Research Scientist)
Yoshiyuki Kajikawa (Research Scientist)
Seiya Nishizawa (Research Scientist)
Hisashi Yashiro (Research Scientist)
Yoshiaki Miyamoto (Postdoctoral Researcher)
Tatsuya Seiki (Postdoctoral Researcher)
Tsuyoshi Yamaura (Postdoctoral Researcher)
Yousuke Sato (Postdoctoral Researcher)
Ryuji Yoshida (Research Associate)
Mamiko Hata (Technical Staff)
Hiroaki Miura (Visiting Researcher)
Sachiho Adachi (Visiting Researcher)
Mizuo Kajino (Visiting Researcher)
Tomoko Ohtani (Assistant)
Keiko Muraki (Assistant)

2. Research Activities

Our research team conducts the pioneering research work to lead the future climate simulation. In order to enhance the reliability of climate model more, we aim to construct a new climate model based on the further theoretically physical principles. Conducting such a model needs tremendously large computer resources. Therefore, it is necessary to design the model to pull out the capability of computers as much as possible. Recent development of supercomputers has a remarkable progress. Hence new numerical techniques should be needed under the collaboration of hardware research and software engineering for the effective use of them on the future HPC, including K computer.

For the above research purpose and background, our team is cooperating with the computational scientists in other fields and computer scientists. We enhance the research and development for the future climate simulations including effective techniques; we make a next-generation climate model. The establishment of the above basic and infrastructure research on K Computer is strongly required, because this research leads to post K (Exa) computer or subsequent ones in the future.

We have been continuing to conduct five ongoing projects and started one project from this fiscal year.

1. Construction of a new library for climate study:
   We have proposed the subject "Estimation of different results by many numerical techniques and their combination" as a synergetic research to MEXT in 2011 through the discussion with the Strategic 5 fields (SPIRE).
2. Grand challenge run for sub-km horizontal resolution run by global cloud-resolving model:
   In order to achieve an outstanding simulation on K computer in climate field, our team are conducting and analyzing the simulation with super-high resolution. This work are done in cooperation with the SPIRE3.
3. Feasibility study of Exa-scale computing using the general circulation model:
   The project of G8 Research Councils Initiative "ICOMEX" has been started from 2011 autumn. Through this project, a part of our team does the feasibility study of Exa-scale computing by the global cloud resolving model and conduct the inter-comparison between the existing icosahedral models.
4. Feasibility study to the future HPCI:
   In order to clarify what can be contributed from computational science to the socio/scientific field, "the Feasibility Study to the future HPCI" funded by MEXT has started from this fiscal year. RIKEN/AICS are now leading the investigation of contribution from the application side. The executive office was established in our team. We are organizing the application community of computational sciences.
5. Disaster prevention research in establishment of COE project:
   Hyogo-Kobe COE establishment project has accepted 5 subjects in 2012. One of subjects is "the computational research of disaster prevention in the Kansai area". In this subject, one of sub-subjects is "Examination of heavy-rainfall event and construction of hazard map", which our team is responsible of.

3. Research Results and Achievements

3.1 Construction of a new library for climate study

SCALE library development

We are working on research and development of a library (named SCALE) for numerical models in fluid dynamical field especially in meteorological field. We examined feasibility of numerical scheme and methods and developed new ones which are suite on massive parallel computers especially K computer. In order to validate the schemes and test their performance in

atmospheric simulations, we have been developing an atmospheric large-eddy simulation model (named SCALE-LES) as a part of the SCALE library. The SCALE library and the SCALE-LES model are currently available as open source software at our web site (http://scale.aics.riken.jp/). It is also installed on K computer and is available for K computer users as an AICS Software (http://www.aics.riken.jp/en/kcomputer/aics-software.html).

Stratocumulus simulations by SCALE-LES

By using SCALE-LES model, we investigated shallow clouds such as stratocumulus which have important role in energy budget of the Earth through radiative process. Stratocumulus has two types of famous structure: closed- and open-cells. We succeeded to simulate the closed- and open-cells (Fig. 1) with a 35m- (in horizontal) and 5m- (in vertical) resolution simulation. Experimental settings are basically follows the DYCOMS-II RF02 setup (Ackerman et al. 2009).

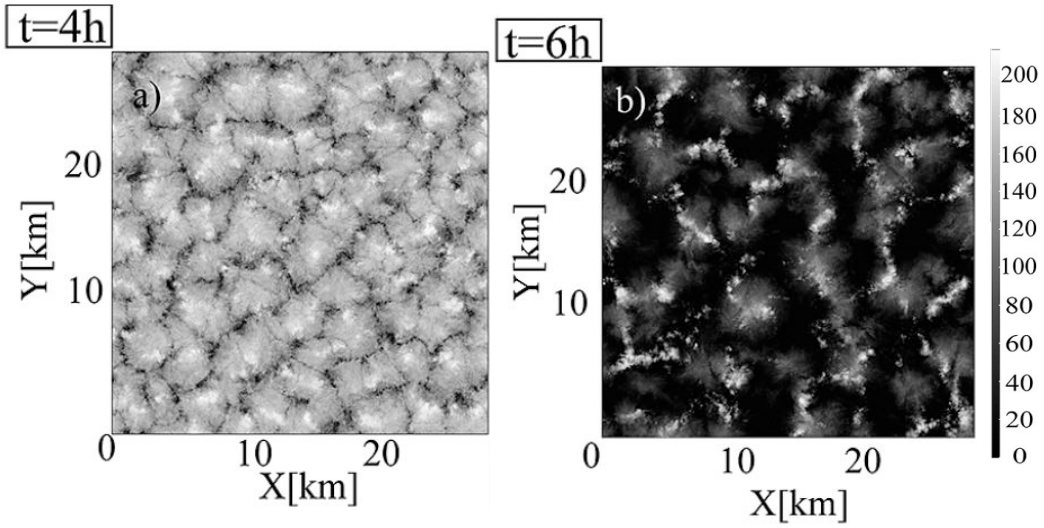


Figure 1. Horizontal distribution of radiance at 660 nm wavelength of simulated stratocumulus at 4 and 6 hours after the start of simulation. (a) Closed- and (b) open-cell structure is well simulated. Unit is W m^{-2} $str^{-1}\mu m^{-1}$.

We plotted the two cloud growth diagrams named Contoured Frequency Optical Depth Diagram (CFODD) and correlation pattern between effective radius (Re) and Cloud Optical Depth (COT) (RE-COT pattern). The former was firstly proposed from the results of satellite remote sensing by Nakajima et al. (2010) and Suzuki et al. (2010) and the latter proposed by Nakajima and Nakjaima (1995). All of them inferred that growth processes of cloud particles can be obtained from the analysis of the CFODD and the RE-COT pattern, but they did not confirm the validity of their inference because satellite remote sensing did not obtain temporal sequence of the CFODD. We also obtained temporal sequence of the CFODD diagram (Fig. 2 a-d) and RE-COT pattern (Fig. 2 e-g). As the result we show temporal evaluation of lifecycle of

individual clouds from non-drizzling mode to drizzling mode and decaying mode. The results supported the inference of the previous studies.

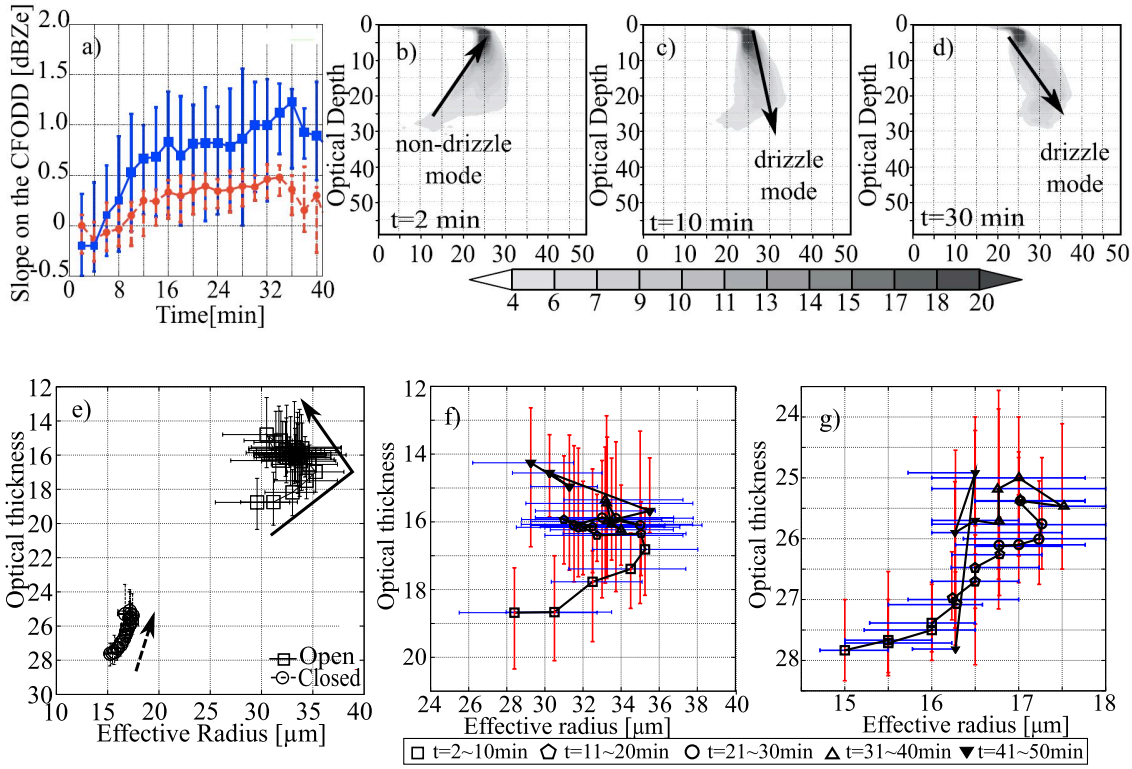


Figure 2. (a) Temporal evolution of the slope of the peak position of radar reflectivity on the CFODD created by the signals of individual clouds in the closed-cell (red line) and open-cell (blue line) cased and the CFODD of individual clouds averaged for all individual clouds in the closed-cell case at (b) t = 2 min, (c) t = 10 min, and (d) t = 30 min after each individual cloud was detected. (e) Trajectory of the center point of each cloud on the RE-COT pattern, averaged for all individual clouds of the open-cell (solid line with open square) and closed-cell (dotted line with open circle) cases, and the same figure but expanded to (f) the open-cell case and (g) closed-cell case at t = 2~10 min (open square), t = 11~20 min (pentagon), t = 21~30 min (circle), t = 31~40 min (closed triangle), and t = 41~48 min (closed triangle). Error bars in (a), (e), (f), and (g) indicate the upper and lower quartiles. The arrow in (b), (c), and (d) indicate the arrow corresponding to non-drizzling and drizzling stages in Fig. 1d, respectively. Arrows in (e) show the direction of movement of the trajectory on the RE-COT pattern.

We compare the cloud growth process obtained from the CFODD and that from the RE-COT pattern. From the comparison, we find that the transition from non-drizzling mode to drizzling mode can be obtained more efficiently from CFODD than from RE-COT pattern. We inferred that the difference is derived from difference of the information used for creating the diagrams. Vertical information included in CFODDs is important for obtaining cloud growth process. This

inference suggests that vertical information of inner cloud should be obtained from next generation satellite (e.g. Himawari-8, Himawari-9). This is an example of the contribution of computational science to cloud and aerosol science, and indicates that numerical simulations can be used to augment satellite observations.

3.2 Grand challenge run for sub-km horizontal resolution run by global cloud-resolving model

Improvement of the performance of NICAM on the K computer

We continue development for both scientific and computational performance improvement of atmosphere model. NICAM (Nonhydrostatic Icosahedral Atmospheric Model) is the global model in out target application. We achieved 10% of performance efficiency/PEAK of NICAM on the K computer with the small number of nodes. The detail is reported in the last year. Here we show a result of strong scaling test in Fig.3. The problem size of the test is about 260 billion grid, which means 14km of horizontal grid spacing, 94 of vertical layer (the layer thickness is 100-300m at the troposphere). NICAM has the parameter for the gird division level (glevel) and region (node) division level (rlevel). The number of horizontal grid is determined by (2^(glevel-rlevel)+2)^2 x 10x4^rlevel/process. The result shows good speedup from 80 nodes (glevel=9, rlevel=2, number of horizontal grid is 16900gridx2/node) to 2560 nodes (1156grid/node) of the K computer. However, the effective speedup was not provided using more nodes. This is because the ratio of the communication time increases in comparison with floating-point operation time. The communication time occupies 5% and 25% of main loop in 80 nodes and 2560 nodes, respectively. The ratio reaches over 50% in 20480 nodes (324grid/node) and 81920 nodes (100grid/node). Further improvement of strong scaling is necessary for the climate simulation, which requires O(10^5) - O(10^7) of steps. The challenges of development are reduction of the communication frequency and reduction/concealment of packing/unpacking cost.

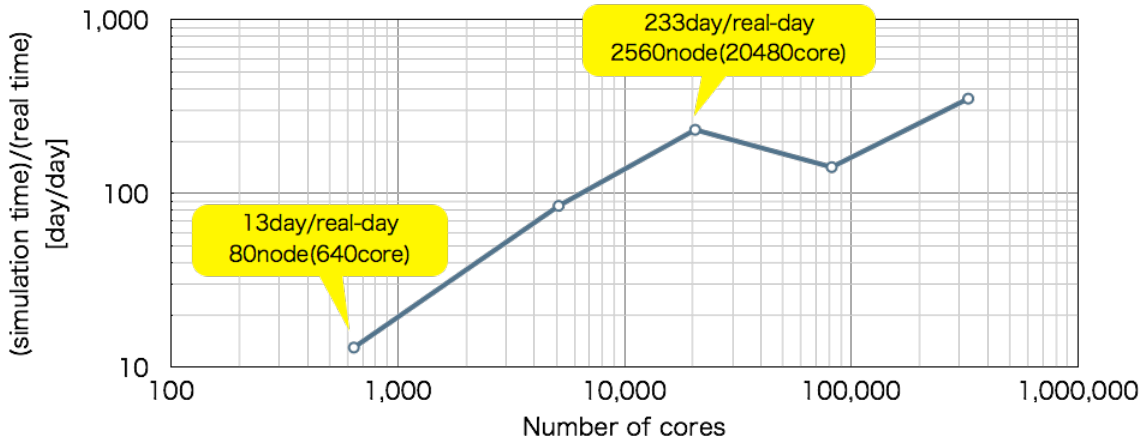


Figure 3. A result of strong scaling experiment on the K computer.

Analysis of global sub-km experiment

We have performed a simulation of global atmosphere with the world-highest resolution (the grid spacing is 870 m) using NICAM. The overview of the simulation has been reported in the last year. We have published a research paper in September 2013, which first succeeded in describing the mean structure of the deep moist atmospheric convection on the globe.

Based on this research, we further conducted an analysis focusing on the convection existing in various cloudy disturbances that cause severe natural disasters such as a typhoon. By considering four representative disturbances: Madden-Julian Oscillation (MJO), Tropical Cyclone (TC), Mid-latitudinal Lows (MDL) and Fronts (FRT) (see Fig.4), we found that the convection in the tropical disturbances (MJO and TC) has tall structure in contrast to that in the mid-latitudinal disturbances (MDL and FRT). More specifically, the MJO convection is strong and formed by large convective available potential energy (CAPE), whereas that in TC is weak and forced by strong low-level convergence. The convection in MDL and FRT is characterized by strong vertical wind shear that approximately correspond to large temperature gradient in the meridional direction. The findings provide useful information for development of cumulus parameterization and better understanding of interaction between the convection and disturbances.

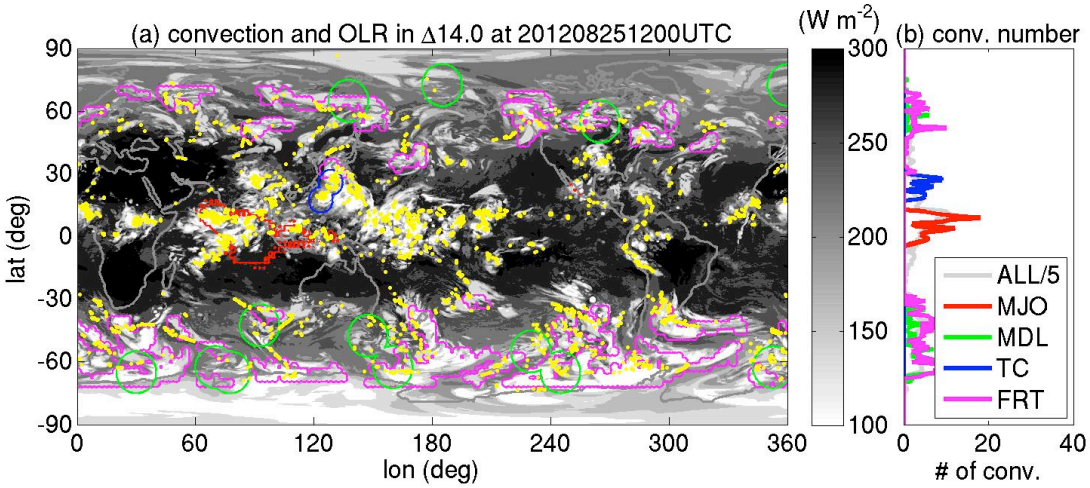


Figure 4. (a) Global distribution of the detected cloudy disturbances and convection overwritten on the Outgoing Longwave Radiation (OLR) in the simulation (gray shaded). The red, blue, green, and magenta contour represents MJO, TC, MDL and FRT, respectively. (b) The latitudinal distribution of convection numbers.

3.3 Feasibility study of Exa-scale computing using the general circulation model

ICOMEX project

The aim of the ICOsahedral-grid Models for Exascale Earth system simulations (ICOMEX) project is development the climate models, which have an efficient computational performance and

provide better scientific result of the simulation. This project is the international activity for the exa-scale computing. We performed inter-model comparison between four participated models as one of the programs of ICOMEX project. The four models, DYNAMICO (France), ICON (Germany), MPAS (US/UK) and NICAM (Japan), are evaluated by four ideal test cases of atmospheric simulation. Computational performances of those models are also measured.

The atmospheric test cases are as follows: baloclinic wave test, long-term global circulation experiment, aqua planet experiment and CMIP5-AMIP experiment. The First test is a deterministic case and the representability of the model compared to the analytical solution is evaluated. The result shows that all models reproduced expected wave pattern (See Fig.5). A detailed error analysis showed that the enhancement of the spatial resolution contributes to the accuracy. The second case is performance test of dry dynamical core (i.e., no water vapor and moist thermodynamics) of the model. The climatological state after the long-term simulation is evaluated statistically. NICAM and ICON were used for this test and the result was compared each other. From the analysis of kinetic energy spectra and wave activity, the spectrum derived from both models showed almost good agreement with the expected spectrum. However, different characteristics were seen in the high wavelength. These results suggest that not only the horizontal grid spacing but also the magnitude of the artificial numerical diffusion term is important factor to the model's "effective" resolution.

For the computational performance, the measurement result of each model mentioned that efficient usage of the memory, especially the memory bandwidth is the important issue. The knowledge provided from this project will contribute the development of the model of each research group. Continuous and wide evaluation is needed for the improvement of climate model from now on.

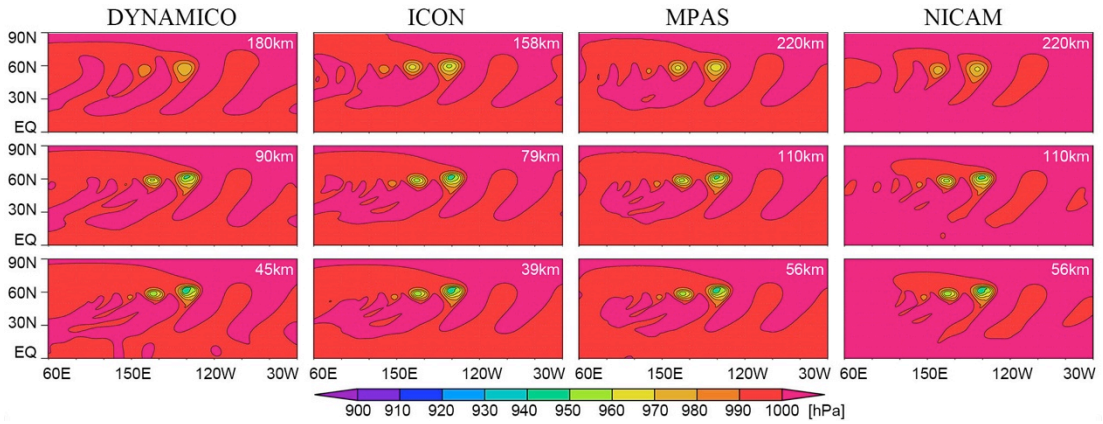


Figure 5. The simulation result of baloclinic wave test. Contour and color shows the surface pressure at the 9th day from initial state. The panels indicate the result of four model and three horizontal grid spacing.

NICAM-DC

Prior to the integration to our new library, we released a part of NICAM as an open source. The name of the package is NICAM-DC. The URL of the web site is http://scale.aics.riken.jp/nicamdc/. The dynamical core and the model framework are included in this package. The package also has the test case to evaluate the scientific performance of the model. The knowledge from the evaluation work in the ICOMEX project was used for the development of the test system. NICAM-DC is used as the benchmark and test-bed and mini-application in the fields of the computational science. For example, several groups of "the Feasibility Study to the future HPCI" used NICAM-DC to evaluate the performance of the kernel on their architectures.

3.4 Feasibility study to the future HPCI

FY2013, 6 general meetings were held and we extracted the social/science subjects, which should be resolved in the next generation HPC. We also discussed about them with the other communities. The "Road map of computational science" is published. The report including the road map can be found at http://hpci-aplfs.aics.riken.jp/ .

3.5 Hoygo-Kobe COE establish project

We succeeded to add the land-surface scheme and topography process to SCALE-LES and validate the each new scheme through several atmospheric simulations. In parallel with the SCALE-LES development, we have examined the heavy rainfall event in the Kobe city. Large amount of the rainfall is shown in June, while the rainfall intensity in June is relatively weaker than other month in boreal summer. We suggest the frontal disturbance is dominant in the rainfall event in June. On the other hand, convective heavy rainfall events are found in August and September. We performed model simulation of three heavy rainfall events in Kobe, 1) fontal rainfall, 2) convective rainfall, 3) combinational effect of typhoon and autumnal rain front by using Weather Research and Forecasting model (WRF). We confirmed the distribution of precipitation cell in the simulations and found the difficulty of simulating the developing process of precipitation cell and its temporal timing. We also conducted the climatological run during boreal summer in 2006-2013 and found the rainfall bias is shown along the mountain area. These preliminary experiments by WRF become reference to the SCALE-LES simulations in the future.

We also have regular meeting for comprehensive disaster-preparedness with Kobe University, Kansai University and public administration of Kobe City and Hyogo Prefecture, approximately once a two month.

4. Schedule and Future Plan

In the next year, we will continue to develop and update the numerical library for K computer.

At the same time, we will give an insight into what kind of the time integration method is promising on K computer and future HPC from the viewpoints of computational and physical performances. Through this project, we will organize and lead the meteorological numerical community for common library towards the post-Peta scale computing.

We especially focus on enhancing the SCALE-LES enough to simulate the atmosphere under realistic condition. Urban canopy process and several experimental tools will be incorporated in the model and validated with the moist convection case. On the COE establishment project, we have a plan to use this SCALE library to simulate the heavy rainfall in Kobe toward to the new-staged hazard map for local severe rain and floods.

We also challenge to figure out the transition process of two types of stratocumulus, open-cell and closed-cell by using SCALE-LES on K computer. Better simulation of these two clouds will bring massive progress not only for robustness of SCALE library but also for better understating of lower cloud. Latter can be applied to global climate modeling in the near future.

Grand challenge run by NICAM will be also continued in cooperation with 3rd Strategic Field Project. The statistical properties of deep convection in the different climatological disturbances will be summarized. Temporal evolution of each convection will be focused in detail.

We will also contribute to the CREST, Strategic Basic Research Programs “Innovating "Big Data Assimilation" technology for revolutionizing very-short-range severe weather prediction” to develop the main climatological model in SCALE library.

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] Sato, Y., S. Nishizawa, H. Yashiro, Y. Miyamoto, and H. Tomita, 2014: Potential of Retrieving Shallow-Cloud Life Cycle from Future Generation Satellite Observations through Cloud Evolution Diagrams: A Suggestion from a Large Eddy Simulation. SOLA, Vol10, pp. 10-14, doi:10.2151/sola.2014-003.

[2] Miyamoto, Y., M. Satoh, H. Tomita, K. Oouchi, Y. Yamada, C. Kodama and J. Kinter III, 2014: Gradient wind balance in tropical cyclones in global nonhydrostatic model simulations. Mon. Wea. Rev., 2014 ; e-View, http://dx.doi.org/10.1175/MWR-D-13-00115.1

[3] Yoshida, R., Y. Kajikawa and H. Ishikawa, 2014: Impact of Boreal Summer Intraseasonal Oscillation on Environment of Tropical Cyclone Genesis over the Western North Pacific. Scientific Online Letters on the Atmosphere, Vol. 10, pp15–18, doi:10.2151/sola.2014-004

[4] Sato, Y., S. Nishizawa, H. Yashiro, Y. Miyamoto, T. Yamaura and H. Tomita, 2014;

Development of a fully compressible Large Eddy Simulation Model, and simulations of stratocumulus life cycle – Contribution from the computational science to science of aerosol and cloud microphysics). Teionkagaku, 72, pp. 265-283.

[5] Iga, S., and H. Tomita, 2013: Improved smoothness and homogeneity of icosahedral grids using the spring dynamics method. J. Comp. Phys.

[6] Blackburn, M., D. L. Williamson, K. Nakajima, W. Ohfuchi, Y. O. Takahashi, Y.-Y. Hayashi, H. Nakamura, M. Ishiwatari, J. McGregor, H. Borth, V. Wirth, H. Frank, P. Bechtold, N. P. Wedi, H. Tomita, M. Satoh, M. Zhao, I. M. Held, M. J. Suarez, M.-I. Lee, M. Watanabe, M. Kimoto, Y. Liu, Z. Wang, A. Molod, K. Rajendran, A. Kitoh, and R. Stratton, 2013: The Aqua-Planet Experiment (APE): Control SST simulation. J. Meteor. Soc. Japan, 91A, 17-56, doi:10.2151/jmsj.2013-A02.

[7] Williamson, D. L., M. Blackburn, K. Nakajima, W. Ohfuchi, Y. O. Takahashi, Y.-Y. Hayashi, H. Nakamura, M. Ishiwatari, J. McGregor, H. Borth, V. Wirth, H. Frank, P. Bechtold, N. P. Wedi, H. Tomita, M. Satoh, M. Zhao, I. M. Held, M. J. Suarez, M.-I. Lee, M. Watanabe, M. Kimoto, Y. Liu, Z. Wang, A. Molod, K. Rajendran, A. Kitoh, and R. Stratton, 2013: The Aqua-Planet Experiment (APE): Response to changed SST profile. J. Meteor. Soc. Japan, 91A, 57-89, doi:10.2151/jmsj.2013-A03.

[8] Miyamoto, Y. and Y. Kajikawa, R. Yoshida, T. Yamaura, H. Yashiro and H. Tomita, 2013: Deep moist atmospheric convection in a sub-kilometer global simulation. Geoph. Res. Lett., doi:10.1002/grl.50944.

[9] Seiki, T., and T. Nakajima 2013: Aerosol effect of the condensation process on a convective cloud simulation, J. Atmos. sci.,. doi: 10.1175/JAS-D-12-0195.1.

[10] Yamaura. T., Y. Kajikawa, H. Tomita and M. Satoh, 2013: Possible impact of a tropical cyclone on the northward migration of the Baiu frontal zone, SOLA, 9, 89-93, doi:10.2151/sola.2013-020.

[11] Lee, S. -S., J.-Y. Lee, K. -J. Ha, B. Wang, A. Kitoh, Y. Kajikawa and M. Abe, 2013: Role of the Tibetan Plateau on Climatological Annual Variation of Mean Atmospheric Circulation and Storm Track Activity, J. Climate, 26, 5270-5286, doi: 10.1175/JCLI-D-12-00213.1.

[12] Yoshida R. and H. Ishikawa, 2013: Environmental Factors Contributing to Tropical Cyclone Genesis over the Western North Pacific. Mon. Wea. Rev., 141, 451-467.

[13] Miyamoto, Y. and T. Takemi, 2013: A transition mechanism for the spontaneous axisymmetric intensification of tropical cyclones. Journal of the Atmospheric Sciences, 70, 112-129.

[14] Tomita, T., T. Yamaura, and Y. Kuwazuru, 2013: Decadal-scale modulation of atmospheric circulation change at the onset of the western North Pacific summer monsoon. SOLA, 9, 161-165.

[15] Nishizawa, S., Y. Sato, H. Yashiro, Y. Miyamoto, R. Yoshida and H. Tomita, Team SCALE, 2013:

Development of atmospheric LES model for large-domain and high-resolution experiments, Nagare, 32, 149-152.

(2) Invited Talks

[16] Tomita, H., Global cloud permitting model, ECMWF annual seminar on Recent developments in numerical methods for atmosphere and ocean modeling, September 2-5, 2013 (Invited)

[17] Kajikawa. Y., Interdecadal Change of the South China Sea Summer Monsoon Onset, 5th THORPEX and S2S Workshop, Jeju, Korea, November 4-5, 2013 (Invited).

(3) Posters and Presentations

[18] Yoshiaki Miyamoto and Tetsuya Takemi, A Triggering Mechanism for the spontaneous axisymmetric intensification of tropical cyclones, 2014 Ocean Science Meeting, Honolulu, Hawaii USA, 2014/2/27.

[19] Yoshiaki Miyamoto, Yoshiyuki Kajikawa, Ryuji Yoshida, Tsuyoshi Yamaura, Hisashi Yashiro, and Hirofumi Tomita, Deep moist convection in a sub-kilometer global simulation, International Workshop on Climate System Modeling, Honolulu, Hawaii USA, 2014/3/10.

[20] Yoshiaki Miyamoto, Richard Rotunno, and George Bryan, An analytical model of maximum potential intensity for tropical cyclones incorporating the effect of ocean mixing, 31st Conference on Hurricanes and Tropical Meteorology, San Diego, California USA, 2014/3/31.

[21] Yoshiaki Miyamoto and Tetsuya Takemi, A Triggering Mechanism for the spontaneous axisymmetric intensification of tropical cyclones, 31st Conference on Hurricanes and Tropical Meteorology, San Diego, California USA, 2014/4/3.

[22] Yousuke Sato, Seiya Nishizawa, Hisashi Yashiro, Yoshiaki Miyamoto and Hirofumi Tomita, Sensitivity of cloud microphysical scheme in SCALE-LES, Climate 2014, Honolulu, USA, 2014/3/11.

[23] Tomita, H., Report on Feasibility Study on Future HPC Infrastructure I, 1st International Workshop on Strategic Development of High Performance Computers, Tsukuba, March 18-19, 2013.

[24] Kajikawa, Y., Advanced Asian summer monsoon onset in recent decades,5th WMO International Workshop on Monsoons (IWM-V), Macao, China, October 28 – November 1, 2013.

[25] Kajikawa. Y., T. Yamaura, H. Tomita and M. Satoh, Possible Impact of a Tropical Cyclone on the Northward Migration of the Baiu Frontal Zone, 6th China-Korea-Japan Joint Conference on Meteorology, Nanjing, China, October 24-25, 2013.

[26] Kajikawa. Y., T. Yamaura, H. Tomita and M. Satoh, Indian summer monsoon onset in 2012 simulated by global cloud-system resolving model NICAM, Davos Atmosphere and

Cryosphere Assembly 2013, Davos, Switzerland, July 8-12, 2013.

[27] Kajikawa, Y., Advanced Asian summer monsoon onset in recent decades, Davos Atmosphere and Cryosphere Assembly 2013, Davos, Switzerland, July 8-12, 2013.

[28] Yashiro, H., H. Tomita and M. Satoh, NICAM simulations on the K computer: recent performance and activities toward to the exascale computing, 15th International Specialist Meeting on the next-generation of climate models and knowledge discoveries through the extreme high-performance simulations and big data, Berkeley CA, USA, March 20-22. 2013

[29] Nishizawa, S., H. Yashiro, Y. Sato, Y. Miyamoto and H. Tomita, Research and Development of Common Basic Library and Environment for Weather and Climate Prediction Models, 15th International Specialist Meeting on the next-generation of climate models and knowledge discoveries through the extreme high-performance simulations and big data, Berkeley CA, USA, March 20-22. 2013.

[30] Miyamoto, Y. and T. Takemi, 2013: A transition mechanism for the spontaneous axisymmetric intensification of tropical cyclones. Japan Geophysical Union 2013, Chiba, Japan, April 28-May 2, 2013.

[31] Yamaura, T. and T. Tomita, 2013: Persistence and the change of Baiu precipitation anomalies. Davos Atmosphere and Cryosphere Assembly 2013, TU-62_B4.1, 8-12 July, Davos, Schweiz.

[32] 佐藤陽祐、八代尚、西澤誠也、宮本佳明、富田浩文、Team-SCALE、計算科学から貢献する雲の本質的理解へ向けた将来展望、日本気象学会春季大会(招待講演)、東京、5 月 2013 年。

[33] 宮本佳明、梶川義幸、吉田龍二、八代 尚、山浦 剛、富田 浩、2013: 深い湿潤対流の解像度依存性—全球 30km から 800m までの解像度感度実験—、日本気象学会 2013 年度春季大会、東京、2013 年 5 月 26 日。

[34] 西澤誠也、佐藤陽祐、八代尚、宮本佳明、富田浩文、Team SCALE、2013: 高解像度重力流実験でみられた不安定のフラクタル構造とそれによる混合、日本気象学会 2013 年度春季大会、東京、2013 年 5 月 18 日。

[35] 山浦剛、梶川義幸、富田浩文、佐藤正樹、2013：梅雨前線帯の北進に対する台風の寄与、日本気象学会 2013 年度春季大会、東京都渋谷区　国立オリンピック記念青少年総合センター、2013/05/16。

[36] 山浦剛、冨田智彦、2013：梅雨降水偏差の持続性とその変化、日本地球惑星科学連合 2013 年大会、千葉県千葉市　幕張メッセ国際会議場、2013/05/24。

[37] 山浦剛、冨田智彦、2013：梅雨前線帯における降水偏差の持続性、日本気象学会 2013 年度秋季大会、宮城県仙台市　仙台国際センター、2013/11/19。

[38] 宮本佳明, 竹見 哲也, 2013: A Triggering Mechanism for the spontaneous axisymmetric intensification of tropical cyclones, 台風セミナー2013, 京都, 2013/10/22。

[38] 佐藤陽祐，八代尚，西澤誠也，宮本佳明，富田浩文，Team-SCALE、2013: Numerical simulations of stratocumulus off the west coast of California, 神戸, 2013/2/28。

[39] 佐藤陽祐、五藤大輔、八代尚、Tran Thi Ngoc Trieu, 富田浩文、中島映至、2013：エアロゾル輸送モデルおよび大気化学輸送モデルを組み込んだ JMANHM による関東域でのシミュレーション、2013 年日本気象学会秋季大会、仙台、2013/11/19。
[40] 富田浩文　2013：「文部科学省 将来の HPCI システムに関する調査研究」報告「アプリケーション分野からみた将来の HPCI システムのあり方の調査研究」、第 10 回戦略的高性能計算システム開発に関するワークショップ、福岡県北九州市、2013/07/30。
[41] 伊賀晋一、2013：熱帯を細かくした格子を用いた水惑星実験、日本気象学会秋季大会、仙台国際センター・仙台、2013/11/19-21。

Complex Phenomena Unified Simulation Research Team

1. Team members

Makoto Tsubokura (Team Leader)
Keiji Onishi (Postdoctoral Researcher)
Chung-gang Li (Postdoctoral Researcher)
Leif Niclas Jansson (Postdoctoral Researcher)
Rahul Bale (Postdoctoral Researcher)
Tetsuro Tamura (Visiting Researcher)
Ryoichi Kurose (Visiting Researcher)
Gakuji Nagai (Visiting Researcher)
Kei Akasaka (Visiting Researcher)

2. Research Activities

The objective of our research team is to propose a unified simulation method of solving multiple partial differential equations by developing common fundamental techniques such as the effective algorithms of multi-scale phenomena or the simulation modeling for effective utilization of the massively parallel computer architecture. The target of the unified simulation is supposed to be complex and combined phenomena observed in manufacturing processes in industrial circles and our final goal is to contribute to enhance Japanese technological capabilities and industrial process innovation through the high-performance computing simulation.

Most of the complex flow phenomena observed in manufacturing processes are relating to or coupled with other physical or chemical phenomenon such as turbulence diffusion, structure deformation, heat transfer, electromagnetic field or chemical reaction. While computer simulations are rapidly spreading in industry as useful engineering tools, their limitations to such coupled phenomena have come to realize recently. This is because of the fact that each simulation method has been optimized to a specific phenomenon and once two or more solvers of different phenomena are coupled for such a complicated target, its computational performance is seriously degraded. This is especially true when we utilize a high-performance computer such as “K-computer”. In such a situation, in addition to the fundamental difficulty of treating different time or spatial scales, interpolation of physical quantities like pressure or velocity at the interface of two different phenomena requires additional computer costs and communications among processor cores. Different mesh topology and hence data structures among each simulation and treatment of different time or spatial scales also deteriorate single

processor performance. We understand that one of the keys to solve these problems is to adopt unified structured mesh and data structure among multiple simulations for coupled phenomena. As a candidate of unified data structure for complicated and coupled phenomena, we focused on the building-cube method (BCM) proposed by Nakahashi[1].

[1]K. Nakahashi, High-Density Mesh Flow Computations with Pre-/Post-Data Compressions, Proc. AIAA 17th CFD Conference (2005) AIAA 2005-4876.
[2] P. L. Roe, Approximation Riemann solver, Parameter Vectors, and Difference Schemes, J. Comput. Phys. 43 (1981) 357-372.
[3] J. M. Weiss and W. A. Smith, Preconditioning Applied to Variable and Constants Density Flows, AIAA. 33 (1995) 2050-2056.

3. Research Results and Achievements

3.1. Development of a very large scale incompressible flow solver with a hierarchical grid system

This year, we have modified the main flow solver for incompressible flow developed last year in the context of its validation in a real development process on the massively parallel environment, including pre- and post-processing. For that purpose, we have utilized real production data (called as dirty CAD) provided by Suzuki Motor Company and Nissan Motor Company and conducted a full-scale vehicle aerodynamics simulation. Finally we have realized the world largest class vehicle aerodynamics simulation based on a real vehicle shape data by using 20 billion numerical cells. At the same time, we have started the accuracy inspection work using the wind tunnel experimental results. This numerical simulation enhanced the companies to utilize the K-computer for their own development purpose and two applications were submitted and accepted for the industrial use projects in FY 2014.

In addition, we have conducted a feasibility study of transient flow simulation around Tokyo station for the possible usage of assessing wind load on high-rise buildings. We will expand this project with the tight collaboration with Tokyo Institute of Technology and some construction companies under the K-computer's general use projects in FY2014.

We are planning to keep developing the software based on this framework in 2014, tackling for improvement of an accuracy of prediction adding numerical functions, physical model, and the tools for the usability improvement.

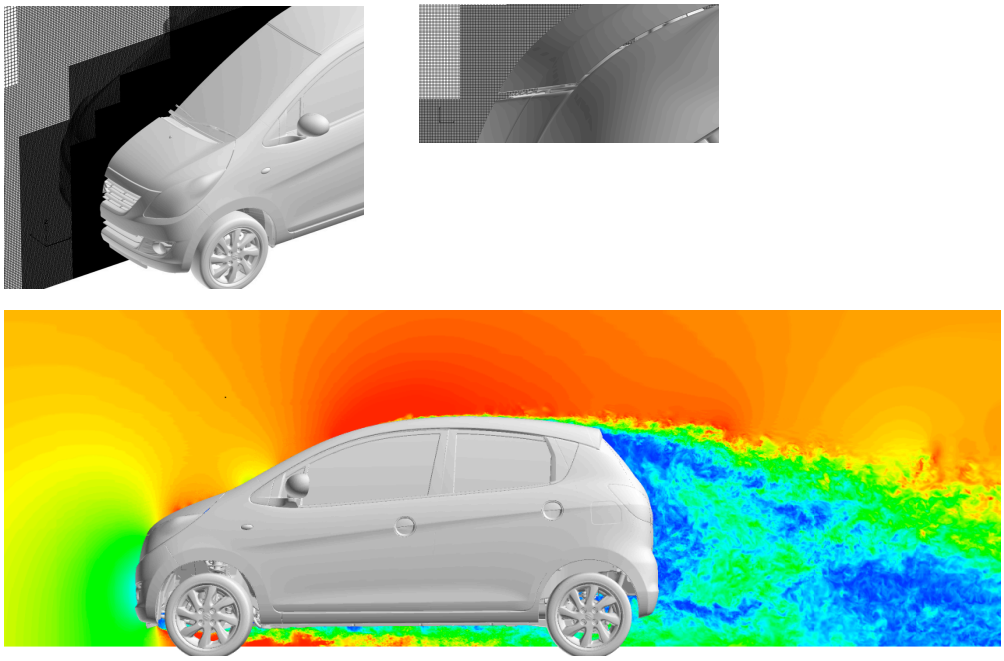
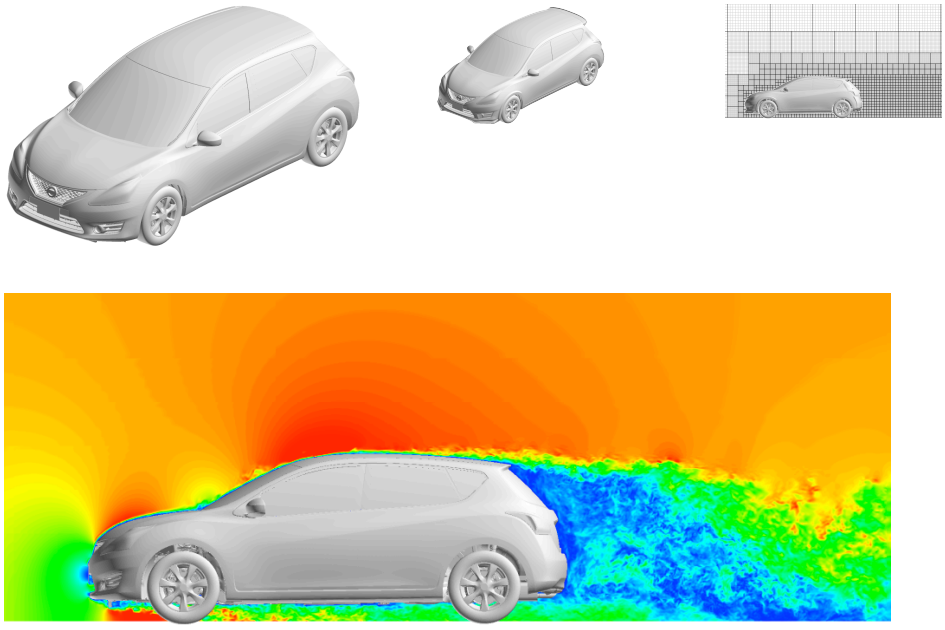


Fig. 1. Practical application of large scale full vehicle aerodynamics simulation using 20 billion cells (Suzuki Motor Company).



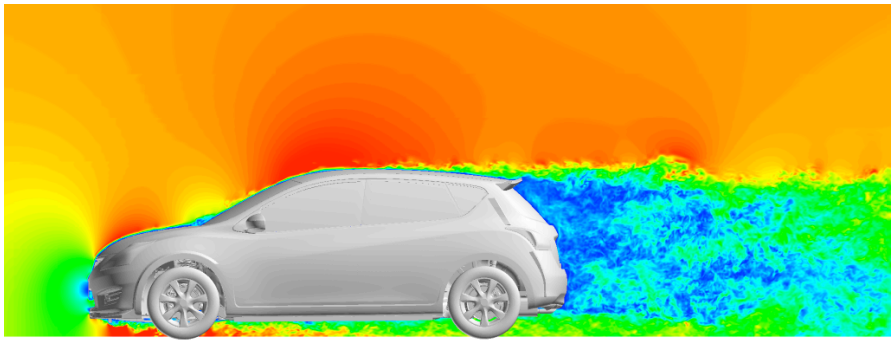


Fig. 2. Analysis of aerodynamic parts effect on full scale vehicle model (Nissan Motor Company).

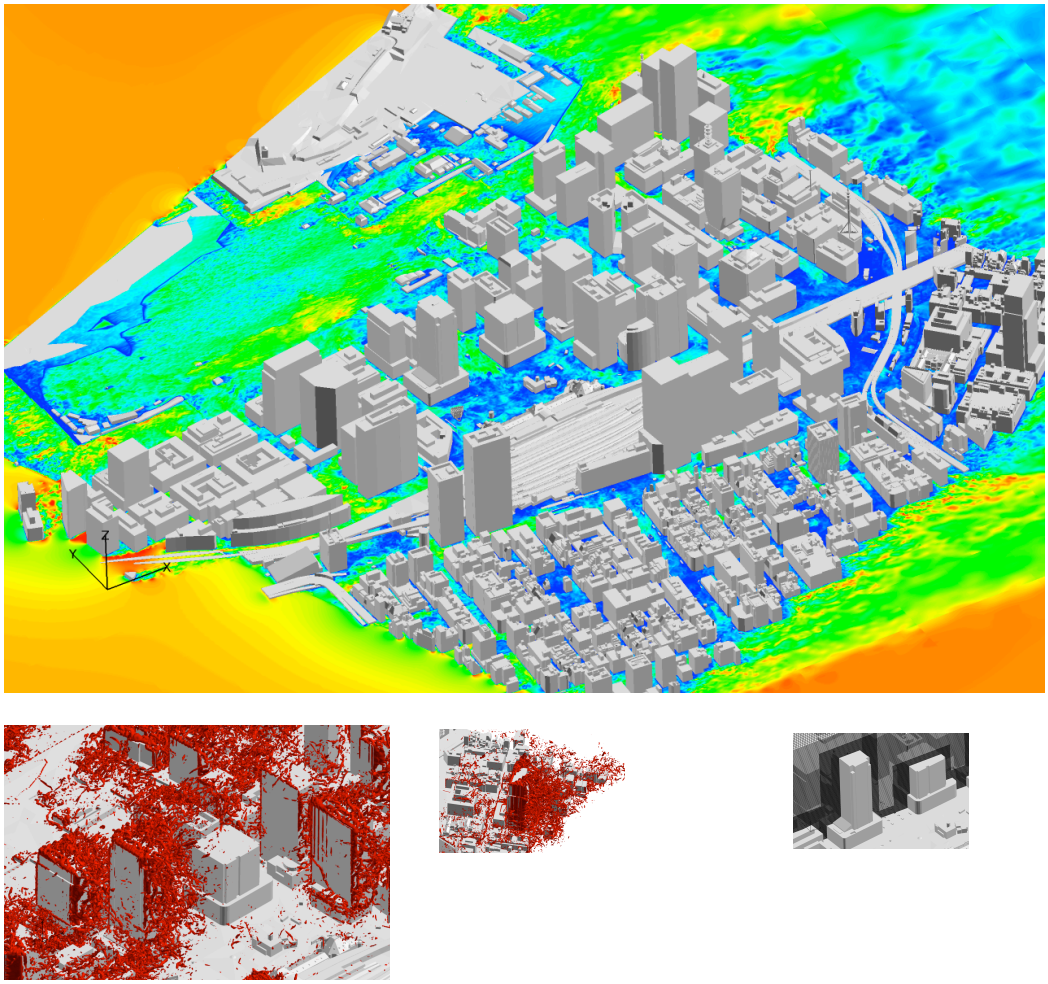


Fig. 3. Wind environment analysis around Tokyo station area.

3.2 Development of unified compressible flow solver for unified low to moderate Mach number turbulence with hierarchical grid system

For the purpose of applying CFD on practical applications, the program with the characteristics of high performance computing, massive parallelization, the ability to handle the complex geometry, suitable from low to high Mach numbers, and adaptability for turbulence is necessary.

Therefore the Roe scheme [2], Weiss and Smith preconditioning method and dual time stepping [3] based on hierarchical data structure have been implemented to unify the solver. Table I shows the weak scaling test of the solver. For 8 CPUs, the peak performance is almost 15% which is much higher than incompressible solver. Additionally, with the increment of the CPUs from 8 to 4096 CPUs, the peak performance just slightly decreases around 1.5% which shows excellent scalability of massive parallelization.

Table I. Weak scaling test.

Nodes	$N_{cube} \times N_x \times N_y \times N_z$	N_{ave}	Elapse time (s)	Data Transfer	Peak(%)
8	$512 \times 16 \times 16 \times 16$	64	54.23	5.03s (9.3%)	14.94
64	$4096 \times 16 \times 16 \times 16$	64	58.99	6.78s (11.5%)	13.74
512	$32768 \times 16 \times 16 \times 16$	64	60.11	6.77s (11.3%)	13.48
4096	$262144 \times 16 \times 16 \times 16$	64	60.12	6.71s (11.2%)	13.48

Immersed boundary is implemented to cope with the complex geometry. Fig. 4 shows the vortex contour around a vehicle at Reynolds number 1000.The flow field disordered by the complex shape and mirror is obvious.

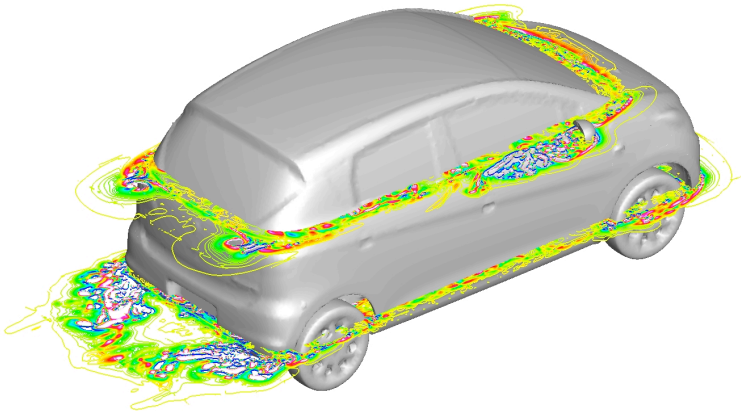


Fig. 4. Vortex contour.

Due to the instinct of the compressible flow, the problem can also be used for our next target: computational aeroacoustics (CAA). The pressure propagation with sine wave in the condition of 30 PPW is conducted and shown in Fig. 5. The comparison with the exact solution is shown in Fig.3. From the Fig. 5, it can be observed that the amplitude keeps decreasing from the pressure

source to the outside. This kind of decay is direct proportion to $P = x^{-0.5}$ and the results in Fig. 6 is in good agreement with the exact solution $P = x^{-0.5}$ when CFL number is smaller than 0.5.

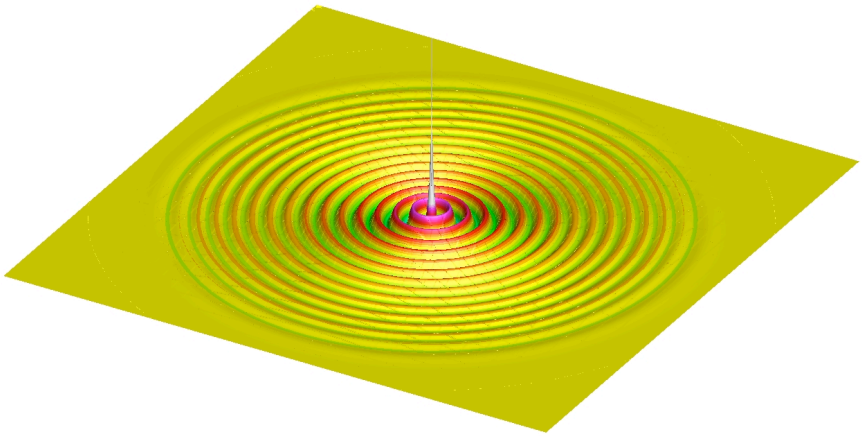


Fig. 5. Pressure propagation with sine wave.

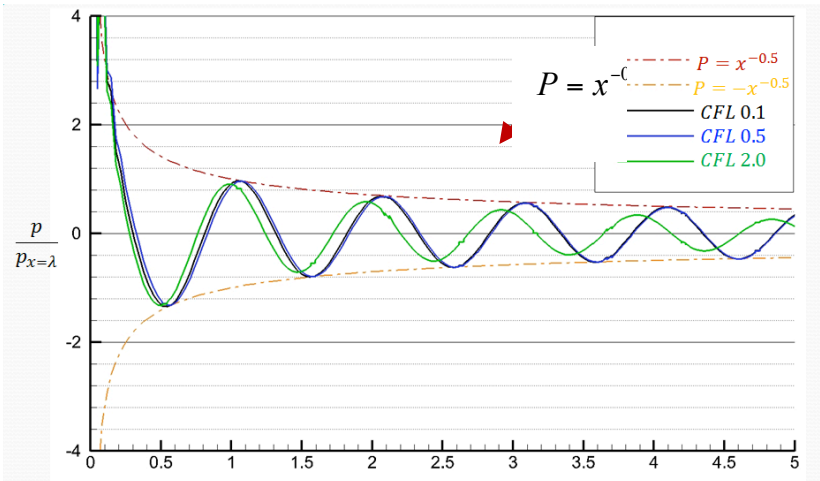


Fig. 6. The comparison with the exact solution.

Based on the present results mentioned above, this unified solver is a sophisticated and powerful tool for practical applications. In order to broaden the suitability on industrial field, the CAA on the vehicle will be conducted for next year.

3.3 Development of a unified framework for incompressible and compressible flow solver

Based on the Building Cube Method (BCM), our unified framework is a merge of the previous flow solvers in our group (incompressible and compressible). Written in modern Fortran 2003, the framework has a modular design, where each solver is an independent module, written by the user or provided by the core library itself. These modules can then be connected together to form a "solver" pipeline, describing the steps necessary to solve a particular multiphysics

problem.

The framework utilize different hybrid parallelization strategies, mainly MPI across nodes together with OpenMP for intra-node parallelism, and MPI I/O for efficient parallel and scalable I/O operations. On a single node our framework achieve around 10-14% of peak flops, and a parallel efficiency of 80-90%, depending on the particular problem at hand (see Fig. 7).

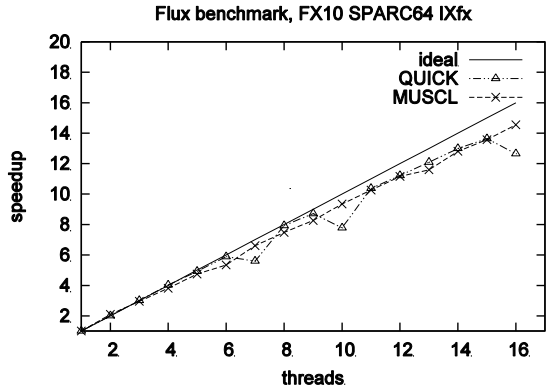


Fig. 7. Single node performance for a incompressible (QUICK) and compressible (MUSCL) scheme.

In order to scale to a large number of MPI tasks we have developed a new multithreaded halo-exchange algorithm. Traditionally, halo-exchange is performed using non-blocking communication, overlapping communication with computation. Our multithreaded approach adds an additional layer on top of this, overlapping packing and sending of communication buffers, performed by one OpenMP thread, with local computation performed in the remaining threads, reducing load imbalance between threads, and improving application performance with up to 20% at scale (see Fig 8.).

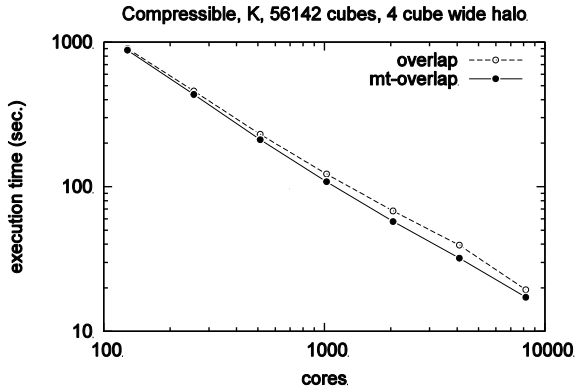


Fig. 8. Execution time for the compressible solver using two different halo-exchange algorithms, the traditional (overlap) and our new multithreaded implementation (mt-overlap).

Our feasibility study of new programming models has also led to the development of a low latency hybrid parallelization of the framework, based on Coarray Fortran together with OpenMP. Furthermore, the framework's modular design allow us to easily interface with routines written in other programming languages, and to target various kinds of current and future accelerators.

3.4 Unified flow and structure simulation based on the immersed boundary methods

Most fluid structure interaction (FSI) problems, encountered in industrial processes and biological systems, involve one or more the following scenarios: Complex motion of structures relative to fluid, motion of structures induced by fluid flow, and deformation of structures induced by fluid forces. Thus, to address FSI problems of practical significance it is necessary to model the afore mentioned scenarios of FSI.

Several approaches for FSI involving deformable and moving structures have been developed over the last four decades. Broadly, these methods fall under two categories Lagrangian-Eulerian (LE) methods and full Eulerian (FE) methods. In LE methods, the structure is represented on a Lagrangian mesh and the fluid on an Eulerian mesh, where as in FE method both structure and fluid are represented on an Eulerian mesh.

The fundamental difference between LE methods and full Eulerian method is the manner of information exchange between fluid and the structure. In LE methods, the information between Lagrangian and Eulerian meshes (i.e. structure and fluid, respectively) is exchanged through operators such as the, so-called, pseudo-delta function. These operators are computationally very expensive and are not suitable for large scale industrial FSI problems. In comparison with LE methods, full Eulerian method does not require any information exchange because both the fluid and the structure are represented on the same Eulerian mesh. Another drawback of LE methods is the issue of load balancing in parallel implementations for moving IB. Moving IB require dynamic load balancing, increasing the difficulty of implementation. Thus, due to lower computational cost and relative ease of implementation, we prefer FE methods over LE methods.

We have adapted the LE based IB method developed by Sharma and Patankar into an FE based IB for Rigid IB dynamics. Through this method we will have the capability to investigate flow induced motion of rigid bodies, flow due to specified motion of rigid bodies as well as flow around immobile rigid bodies. In Fig. 9, as an example of a preliminary test case, the gravity induced motion of a rigid sphere is shown. We use the FE method developed by Sugiyama et al. to model the dynamics of deformable IB. To test our implementation we carried out simulation

of the motion and deformation of a compliant sphere placed in a cavity flow (see Fig. 10).

In FE based IB methods, the IB is represented on the Eulerian mesh through a colour function such as volume of fluid (VOF) or through a level set of a distance function. The position and velocity of the function representing the IB is updated through the hyperbolic advection equation $\frac{\partial f}{\partial t} + \boldsymbol{u} \cdot \nabla f = 0$, where f is either the VOF or the level set function, and $\boldsymbol{u}$ is the fluid velocity field. The accuracy with which sharpness of the IB-fluid interface, and volume and shape of the IB are maintained throughout IB's motion and deformation depends on the advection scheme used for solving the advection equation, and on the type of the function f chosen to represent IB. We are currently doing a literature survey (and testing) of the available advection schemes to find an accurate and inexpensive advection scheme for the equation of motion of the IB.

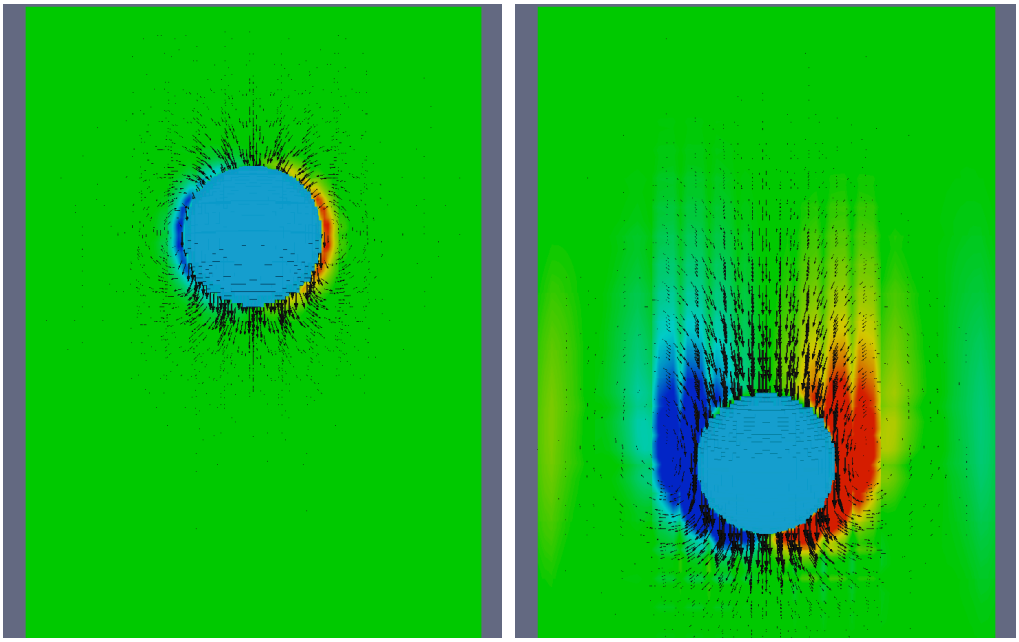


Fig. 9. Gravity induced motion of a rigid sphere at Re = 40. Left: Flow field at t = 0.1 sec. Right: Flow field at t = 1.9 sec. The colour contours represent vorticity and the arrows represent the velocity vector.

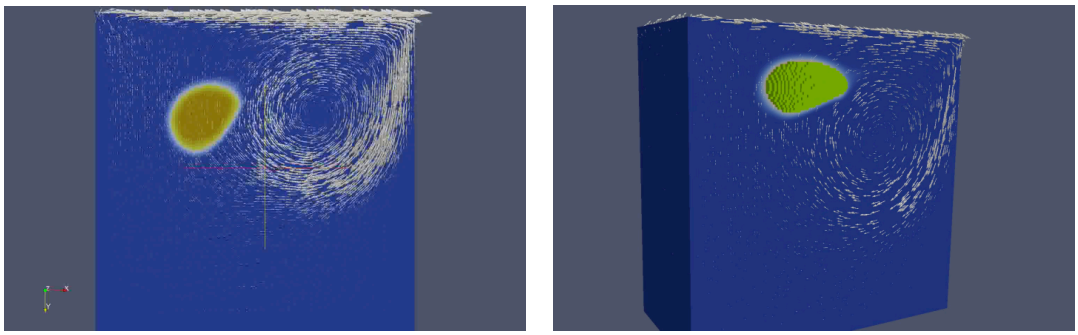


Fig. 10. A compliant deformable sphere place in a cavity flow at Re = 100. Left: Flow field and configuration of the sphere represented on a 2D place through the center of the deformed sphere. Right: Same as left pane but represented in 3D and at a different time instant.

[1] K. Nakahashi, High-Density Mesh Flow Computations with Pre-/Post-Data Compressions, Proc. AIAA 17th CFD Conference (2005) AIAA 2005-4876.

[2] P. L. Roe, Approximation Riemann solver, Parameter Vectors, and Difference Schemes, J. Comput. Phys. 43 (1981) 357-372.

[3] J. M. Weiss and W. A. Smith, Preconditioning Applied to Variable and Constants Density Flows, AIAA. 33 (1995) 2050-2056.

4. Schedule and Future Plan

(1) Five-year objectives and goals toward 2017

a. Construction and development of the simulation technology for bringing out the performance of K computer

b. Proposal of the technological trend of HPC simulation toward EXA-scale

(2) Long-term objectives

a. Establishment of the research and development center for industrial simulation technology

b. Contribution to computer science by expanding the developed simulation technology to different fields

(3) Time schedule

	2012	2013	2014	2015	2016	2017
Proposal of the project	→ Interview to the industry and feasibility study	→ Making specification list for the development				
Building light libraries		→ Library development		→ Porting guideline		
		→ Application development				

Development of the coupling algorithms for the PETA-scale computing			Development of the scaling algorithms Development of the coupling algorithms			
Validation studies			PETA-scale applications		Performance test of the post PETA-scale applications	

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] W. S. Fu*, C. G. Li, M. Tsubokura, Y Huang and J. A. Domaradzki, An Investigation of Compressible Turbulent Forced Convection by an Implicit Turbulence Model for Large Eddy Simulation, Numerical Heat Transfer, Part A: Applications 64 (2013) 858-878.

(2) Conference Papers

[2] 大西 慶治, 坪倉 誠, "階層型直交格子を用いた大規模自動車複雑形状空力解析", 日本機械学会 2013 年度年次大会, (2013).

[3] Onishi, K., Tsubokura, M., “Enhancement of Wall Boundary Condition for Dirty CAD on Building Cube Method based Immersed Boundary”, The 10th International Conference on Flow Dynamics (ICFD2013), (2013).

[4] Onishi, K., Obayashi, S., Nakahashi, K., Tsubokura, M., “Use of the Immersed Boundary Method within the Building Cube Method and its Application to Real Vehicle CAD Data”, AIAA-2013-2713, (2013)

[5] C. G. Li, M. Tsubokura, An implicit turbulence model for Preconditioned-Roe scheme by using Truncated Navier-Stokes Equations, 66th Annual Meeting of the APS Division of Fluid Dynamics.

(3) Invited Talks

[6] M. Tsubokura, “スパコン「京」の産業利用成果”, HPC 産業利用スクール「京」特別コース（スパコン技術産業応用協議会主催）, Jan. 15, 2014.

[7] M. Tsubokura, “「京」コンピュータが可能にする未来の自動車空力シミュレーション”, スーパーコンピュータ「京」を知る集い in 盛岡（理化学研究所主催）, Dec. 7, 2013.

HPC Programming Framework Research Team

1. Team Members

Naoya Maruyama (Team Leader)

Motohiko Matsuda (Research Scientist)

Soichiro Suzuki (Technical Staff)

Mohamed Wahib (Postdoctoral Researcher)

Shinichiro Takizawa (Research Scientist)

2. Research Activities

We develop high performance, highly productive software stacks that aim to simplify development of highly optimized, fault-tolerant computational science applications on current and future supercomputers, notably the K computer. Our current focus of work includes large-scale data processing, heterogeneous computing, and fault tolerance. A major ongoing project in our group will deliver a MapReduce runtime that is highly optimized for the intra- and inter-node architectures of the K computer as well as its peta-scale hierarchical storage systems. Another major project focuses on performance and productivity in large-scale heterogeneous systems. Below is a brief summary of each project.

1) Simplified Parallel Processing with KMR

MapReduce is a simple programming model for manipulating key-value pairs of data, originally presented by Dean and Ghemawat of Google. User-defined map and reduce functions are automatically executed in parallel by the runtime, which in turn enables transparent out-of-core data processing using multiple machines. Our KMR library, which is currently under active development, is similar to the original MapReduce design by Dean and Ghemawat, but its implementation is significantly extended for the node and storage architectures of the K computer. In particular, we exploit the two-level parallel storage systems so that costly data movement can be minimized. Data shuffling in MapReduce is also a subject of optimizations using the 6-D torus interconnect networks.

2) Physis: An Implicitly Parallel Stencil Computation Framework

Physis is a framework for stencil computations that is designed for a variety of parallel computing systems with a particular focus on programmable GPUs. The primary goals are high productivity and high performance. Physis DSL is a small set of custom programming constructs, and allows for very concise and portable implementations of common stencil computations. A single Physis program runs on x86 CPUs, NVIDIA GPUs, and even clusters of them with no

platform-specific code. This software consists of a DSL translator and runtime layer for each supported platform. The translator automatically generates platform-specific source code from Physis code, which is then compiled by a platform-native compiler to generate final executable code. The runtime component is a thin software layer that performs application-independent common tasks, such as management of GPU devices and network connections.

3. Research Results and Achievements

3.1. Simplified Parallel Programming with KMR

1) Kmrshell: A simple building block for MapReduce-style workflow

MapReduce is already a very simple model, but KMR's new functionality "kmrshell", further simplifies parallel programming which can start thousands of Unix commands without coding in C or Fortran. Starting thousands of programs on distinct data sets is a typical scenario of the jobs running on the K computer, but it requires tedious programming if directly implemented with MPI. "Kmrshell" abstracts invocation of multiple Unix commands as mappers and reducers, and efficiently combines their results through pipelining using KMR's high-performance data shuffling. Unmodified sequential or MPI programs can be executed more easily with kmrshell.

2) Automatic affinity-aware large-scale file I/O

KMR implements a new affinity-aware file loading method, which exploits locality information of the files to the I/O nodes [5-(2)-1]. The FEFS filesystem on K is based on file striping, in which a content of a file is segmented to many small chunks and they are scattered across many I/O nodes. It exposes locality of file contents between the I/O nodes and the computing nodes, enabling more efficient accesses to file segments from a near-by computing node, which also minimizes network contention during file loading. The location information of scattering the segments of a file can be obtained by using the system interface to the FEFS filesystem. KMR divides the computing nodes into the groups by the locality to the I/O nodes, and assigns the task of file loading by their affinity to the segments of a file. The following figure shows the improvement achieved by the affinity-aware file loading method.

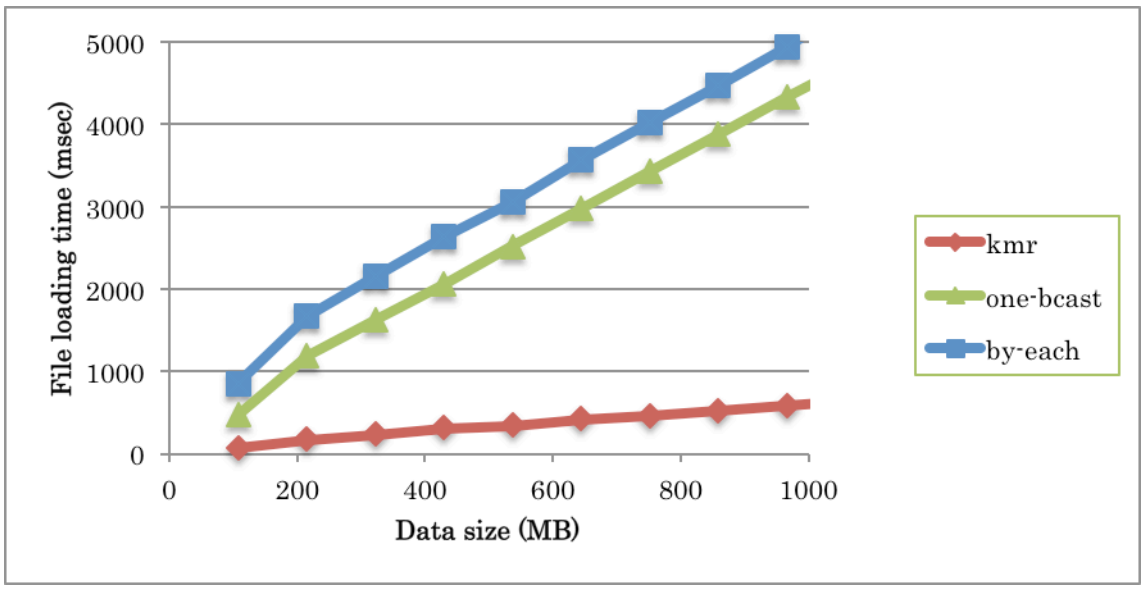


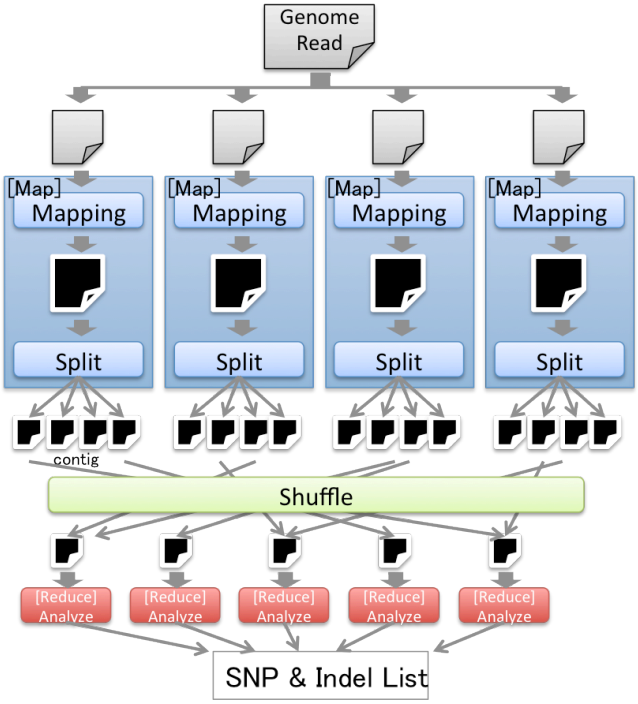
Figure. File loading performance. The line with "kmr" is by affinity-aware file loading. The "one-bcast" is the older method in which one node loads a file and broadcasts it. The "by-each" is a naïve method in which each node loads a file independently.

3) Fault-tolerant MapReduce

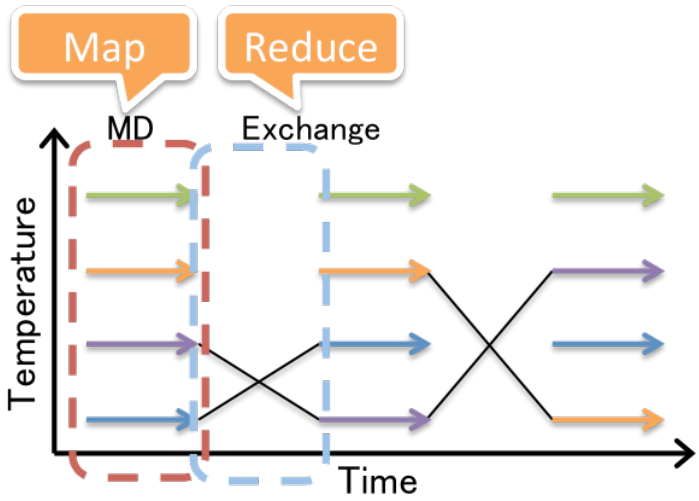
To enable job completion in face of system faults and to enable long term job execution exceeding the maximum elapse time, we implemented a checkpoint/restart feature to KMR. We designed this feature to automatically and transparently perform checkpoint/restart from KMR users. This feature will be included in the next release, which will be available early in FY2014.

4) KMR application examples

As MapReduce is originally designed for data parallel processing, it is easy to apply MapReduce to scientific data analysis [5-(2)-2]. We applied KMR to implement genome analysis, especially to cancer cell's mutations detection. As shown in the following figure, if we split the input genome sequences into small parts we can perform mapping and split them in parallel. This process can be mapped to the Map part of MapReduce. The split results should be merged based on their patterns and it can be mapped to the Shuffle part of MapReduce. The final analysis process can be implemented as Reduce part of MapReduce. KMR also starts to be used to analyzing huge amount of images, more than 1 million/day, generated by SACLA.



MapReduce can be applied to represent certain kind of scientific application's workflows, such as embarrassingly parallel tasks and ensemble simulations. We used KMR to implement Replica-Exchange Molecular Dynamics (REMD), a representative ensemble simulation. REMD is an iterative application that runs MDs in parallel and performs exchange after that in iteration. MapReduce can be applied to represent the iteration where Map runs MDs and Reduces does exchange. KMR starts to be used in AICS research tams to represents their application workflow, such as data assimilation for weather forecasting, social simulation and visualization.



By applying MapReduce to the above applications, application researchers or developers can reduce their coding tasks as MapReduce provides mechanisms for task management, and they can concentrate on implementing the application logics. Furthermore, as KMR is designed especially for the K computer, using KMR will benefit performance on the K computer.

3.2 Physis: An Implicitly Parallel Stencil Computation Framework

One of the main design goals of Physis is to generate high quality code optimized for memory-bound applications on GPU accelerators. A classical optimization technique for increasing memory-bound applications is loop fusion, which translates loops using the same data arrays into a single loop so that accesses to the same data can be reused via on-chip memories such as registers and caches. A similar technique can be applied to GPU applications that consist of a call sequence of GPU-offloaded functions (called kernels in CUDA terminology). By creating a fused kernel that include multiple kernels using the same data arrays, accesses to off-chip DRAM memory can be reduced by exploiting on-chip memories such as GPU shared memory.

We envision that such code transformation technique can be automatically implemented with high-level frameworks such as Physis. The Physis DSL, while limited to stencil computations with regular grids, gives the framework with flexibility in generating any combinations of fused kernels within the constraint of data dependencies among stencils. However, a naive greedy approach to fusing kernels will not be necessarily effective due to the following challenges. First, kernel fusion does not always lead to more efficient code even with shared data being cached at on-chip memories. Other performance-critical architectural constraints, such as the capacity of shared memory, latency to accessing the shared memory, and potential increase of register pressure, need also be carefully considered when deciding fusing a given set of kernels. Furthermore, production applications tend to contain a large number of kernels, much as loops in CPU codes, therefore the number of potential combinations of fusions can be intractably large with simple greedy approaches.

To address the two challenges and achieve speedup by effectively reducing the off-chip memory traffic, we formulate kernel fusion as a combinatorial optimization problem and propose the use of an approximation search heuristic to search the exponentially proportional space of possible fusions.

More specifically, we derive the optimization problem by constructing a data dependency graph and order-of-execution graph for the kernels in the program. Our search heuristic uses a light-weight and accurate projection method of performance upper bound to evaluate the quality of candidate solutions. The upper bound on performance is projected for potential fused kernels without requiring any form of code representation. This light-weight method is essential to enable fusions for applications with a large number of kernels and data arrays.

Our main achievements so far are: a) A formulation of the kernel fusion as an optimization problem, b) The use of a scalable search heuristic to search for near-to-optimal solutions in the space of possible kernel fusions, c) Using a highly accurate codeless upper-bound performance projection to guide KF and, d) Experimental evidence of the effectiveness of the kernel fusion optimization when applied to a test suite and two real world weather applications with tens of kernels and data arrays. As will be shown later, the introduced search method identified the optimal kernels to fuse for the weather applications within a reasonable amount of time. The actual kernel fusion transformation with two climate-modeling applications resulted in more than 1.35x and 1.2x speedup on NVIDIA Kepler GPUs.

4. Schedule and Future Plan

We plan to continue the development of KMR for further simplifying usage of large-scale systems. In particular, our primary focus in the coming years is to optimize I/O intensive applications by further exploiting data locality on the K computer. Toward that end, we will first try to identify common I/O access patterns of the computational science applications running on K, and examine potential improvements of I/O performance by various static and runtime techniques such as runtime code and data migrations. We plan to implement such advanced optimizations with the KMR library so that user applications built using the KMR library can transparently use our optimizations. We also plan to release a new version of KMR with a checkpoint/restart mechanism so that KMR applications can continue execution even in the presence of system failures due to, e.g., hardware faults.

The Physis framework will also be further extended with more advanced code generation techniques such as kernel fusion as presented above. We plan to realize the model-based scalable kernel fusion within the framework so that the performance of stencil applications written in Physis can be further more efficient.

5. Publication, Presentation and Deliverables

(1) Conference Papers

[1] Naoya Maruyama, Takayuki Aoki, "Optimizing Stencil Computations for NVIDIA Kepler GPUs," International Workshop on High-Performance Stencil Computations, Vienna, January 2014.

[2] Shinichiro Takizawa, Motohiko Matsuda and Naoya Maruyama: Supporting Workflow Management of Scientific Applications by MapReduce Programming Model. IPSJ HPCS2014 (2014).

[3] Toshiya Komoda, Shinobu Miwa, Hiroshi Nakamura, Naoya Maruyama, "Integrating Multi-GPU Execution into an OpenACC Compiler," 42nd International Conference on Parallel

Processing (ICPP), pp. 260--269, Lyon, France, October 2013.

[4] Mohamed Attia Wahib, Naoya Maruyama, "Highly Optimized Full GPU-Acceleration of Non-hydrostatic Weather Model SCALE-LES," IEEE Cluster 2013, Indianapolis, IN, USA, September 2013.

[5] Motohiko Matsuda, Naoya Maruyama, Shinichiro Takizawa, "K MapReduce: A Scalable Tool for Data-Processing and Search/Ensemble Applications on Large-Scale Supercomputers," IEEE Cluster 2013, Indianapolis, IN, USA, September 2013.

[6] Tetsuya Hoshino, Naoya Maruyama, Satoshi Matsuoka, Ryoji Takaki, "CUDA vs OpenACC: Performance Case Studies with Kernel Benchmarks and a Memory-Bound CFD Application," Proceedings of the 2013 IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid 2013), Delft, the Netherlands, May 2013.

[7] Mohamed Slim Bouguerra, Ana Gainaru, Leonardo Bautista Gomez, Franck Cappello, Satoshi Matsuoka, Naoya Maruyama, "Improving the Computing Efficiency of HPC Systems Using a Combination of Proactive and Preventive Checkpointing," Proceedings of the 27th IEEE International Parallel and Distributed Processing Symposium (IPDPS'13), Boston, USA, May 2013.

(2) Invited Talks

[8] Naoya Maruyama, "Miniapps for Enabling Architecture-Application Co-design for Exascale Supercomputing," 19th Workshop on Sustained Simulation Performance, Invited Talk, March 2014.

[9] Naoya Maruyama, High performance and high productivity with application frameworks, Kyoto University, Invited talk, July 2013.

(3) Posters and Presentations

[10] Tetsuya Hoshino, Naoya Maruyama, Satoshi Matsuoka, "OpenACC Performance and Optimization Studies With Kernel and Application Benchmarks," GPU Technology Conference, Poster, San Jose, CA, USA, March 2014.

[11] Kento Sato, Akira Nukada, Naoya Maruyama, Satoshi Matsuoka, "I/O Acceleration With GPU for I/O-Bound Applications," GPU Technology Conference, Poster, San Jose, CA, USA, March 2014.

[12] Mohamed Wahib, Naoya Maruyama, "Scalable Kernel Fusion for Memory-Bound GPU Applications," GPU Technology Conference, Poster, San Jose, CA, USA, March 2014.

[13] Mohamed Attia Wahib, Naoya Maruyama, "Scalable Kernel Fusion for Memory-Bound GPU Applications," SIAM Conference on Parallel Processing, MS 49: Parallel Methods and Algorithms for Extreme Computing, Portland, Oregon, USA, February 2014.

(4) Patents and Deliverables

[14] Motohiko Matsuda, Shinichiro Takizawa, Naoya Maruyama, "KMR: A MapReduce Library for K," http://mt.aics.riken.jp/kmr/, 2013.

Advanced Visualization Research Team

1. Team members

Kenji Ono (Team Leader)

Jorji Nonaka (Researcher)

Chongke Bi (Postdoctoral Researcher)

Hamed Khandan (Postdoctoral Researcher)

Kazunori Mikami (Technical Stuff)

Masahiro Fujita (Visiting Researcher)

Kentaro Oku (Visiting Researcher)

Naohisa Sakamoto (Visiting Researcher)

Yukiko Hayakawa (Assistant)

2. Research Activities

The purpose of our visualization team is to construct a parallel visualization environment for large-scale datasets, which are generated from K computer, and to provide the visualization environment for the users. Of course, the development of elemental technologies is included. The following is the objectives of our research in FY2013.

1) Data centric approach for simulation and post-processing (Ono)
2) Development of a visualization technique for large-scale dataset (Nonaka)
3) Data compression for large-scale dataset (Bi)
4) Design of the "A-Cell" portable SIMD framework for heterogeneous computing, development and release of a simulator for visualization and analysis of A-Cell system, and partial development of A-Cell source-to-source compiler (Khandan)

3. Research Results and Achievements

3.1. Data centric approach for simulation and post-processing

Since simulations executed on the K computer often generate large-scale and numerous files, once the data files are generated it is hard to copy or move the data owing to the limitation of the storage. Thus, it is essential for us to manage such many distributed files. We developed an efficient file management library CIOlib using meta-data information so that the library allows us to share the data between different applications such as simulator and post-processing programs. The meta-data is described simple YAML like notation and consists of two types of the information: information related to the parallel process and information related to computed results. This information is described in proc.dfi and index.dfi files respectively. One of the useful functions in developed CIOlib is file loading. The number of execution processes

may vary in some cases, for instance, between simulation and data processing/visualization, or the restart process in simulation. In many cases, file-based data processing after simulation employs much fewer processes than the simulation itself. We consider and provide various file loading patterns for the user's convenience. Figure 1 shows an example of a file loading function that CIOlib provides.

The information included in the proc.dfi can automatically process the following patterns.

a) Normal Loading

The number of processes and the situation of partitioning are the same between the previous and the current session. Most cases choose this pattern.

b) Refinement Loading

In this refinement case as shown in Figure 1, the number of processes is the same; however, the resolution is different. Each process in the current session reads the same file that the process has written in the previous session. However, because the resolution is doubled, interpolation should be performed. User can overload the interpolation method.

c) MxN Loading

M and N denote the number of processes in the previous and current sessions, respectively. Even if M and N are equal but the partitioning is different, the loading pattern becomes MxN loading. Figure 1 shows this pattern for the same resolution, and Figure 1 demonstrates the case of different resolutions and different partitioning. This loading pattern is considerably useful when the user changes the number of processes in a successive simulation process.

d) Staging Assistance

In certain computational environments, the files required for computation need to be transferred from the global file system to the local file system, which is a dedicated disk partition for computations in a batch job, before the calculation begins. This file transfer process is called a stage-in. In the MxN file loading pattern, each current process may need different files that the process wrote in the previous session. In this case, the file that the process needs must be determined prior to submitting a batch job. This procedure is also performed using proc.dfi information. Figure 1 depicts an example. The previous session has M = 9 processes and the current session has N = 4. For instance, the current process of rank 0 (N{0}) demands M{0, 1, 3, 4}. This relationship can be obtained from the information described in proc.dfi.

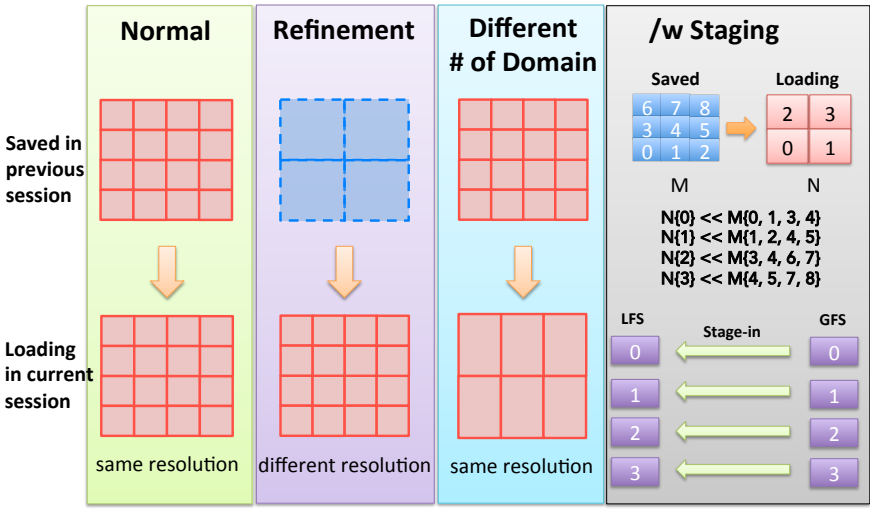


Figure 1. Four file I/O patterns provided by CIOlib.

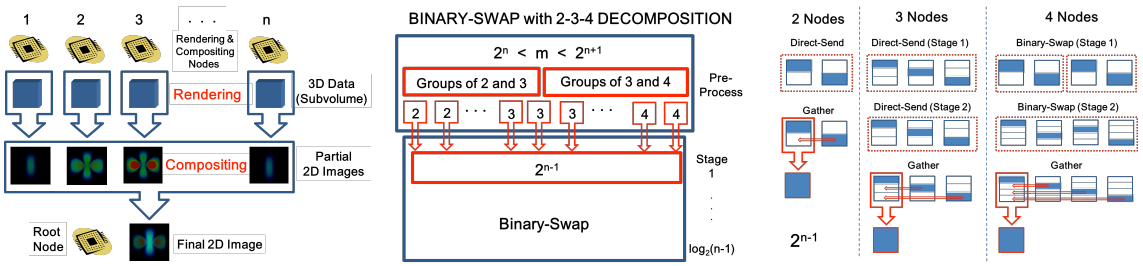
3.2 Development of visualization technique for large-scale dataset

The most popular approach for visualization of large datasets is the sort-last parallel visualization pipeline depicted in Fig. 2a. Most of parallel rendering algorithms are embarrassingly parallel in nature, however the images generated at each rendering node should be composited together to generate the final image. Since it requires interprocess communication among the entire nodes, it usually dominates the total cost of a parallel rendering process. As shown in Fig. 2a, image composition process works coupled with the rendering process, and the same node used for rendering is also used for composition. As a result, the number of rendering nodes determines the number of composition nodes. Although the number of rendering nodes depends on several factors, it is highly important to have a scalable image composition algorithm that works with arbitrary number of nodes.

Parallel image composition has been studied for almost two decades and several algorithms have been proposed so far. Currently, there exist efficient image composition algorithms for power-of-two (2^n) number of nodes. However, when handling non-power-of-two number of nodes, an additional processing is usually applied causing performance penalty. The simplest way is to execute as a pre-processing converting to a power-of-two number of nodes. Since it can be costly, another approach is to distribute this processing overhead to the entire parallel image composition process. As a lightweight pre-processing approach, we investigated the use of 2-3-4 Decomposition method to convert a given non-power-of-two number of nodes to a power-of-two number of nodes. It is worth noting that, in the case of the K Computer, to make full use of the allocated computational resources, multiples of 12 (non-power-of-two) might be

appropriate for job execution.

The 2-3-4 Decomposition works by creating groups of 2, 3 or 4 nodes as shown in Fig. 2b. Considering a non-power-of-two number of composition nodes (m) which is bounded by two power-of-two values, $2^n < m < 2^{n+1}$, when applying 2-3-4 Decomposition, it will create exactly 2^{n-1}, that is, a power-of-two number of groups. By independently compositing each of these groups, as shown in Fig. 2c, it will generate a power-of-two number of images, and by using the local root node at each of these groups it will be possible to apply any of the existing image composition nodes for power-of-two number of nodes. The maximum performance penalty is limited to the overhead of compositing four images. In the case of using Binary-Swap image composition, which is probably the most popular image composition method for power-of-two number of nodes, we verified a stable performance penalty in the range of 1.5 to 1.75 times as those of Binary-Swap on a large-scale image composition environment of up to 32K thousands of composition nodes. It is worth noting that this decomposition method does not depend on any composition parameter to be specified by the user, and has predicable performance behavior. Our ongoing work includes a study to further reduce this performance penalty in certain circumstances.



a) Sort-last parallel visualization pipeline. b) An application of 2-3-4 Decomposition. c) Composition of 2-3-4 groups

Figure 2. 2-3-4 decomposition in sort-last approach.

3.3 Data compression for large-scale dataset

In this year, we have proposed two methods for data compression for large-scale dataset.

Firstly, we proposed a parallel data compression method using POD (Proper Orthogonal Decomposition). However, this method can only deal with the cases that both the number of time steps and the number of processors are power-of-two. Therefore, a 2-3-4 combination method was proposed to resolve the problem of non-power-of-two.

3.3.1. A Study of Parallel Data Compression Using Proper Orthogonal Decomposition

The growing power of supercomputers continues to raise scientists' ability to model larger, more sophisticated problems in science with higher accuracy. Equally important is the ability to make full use of the data output from the simulations to help clarify the modeled phenomena and facilitate the discovery of new phenomena. However, as the scale of computing has grown, there has been a corresponding growth in available data. Outputting most of this data is simply not feasible, which defeats the purpose of conducting large-scale simulations. In order to address this issue so that more data may be collected and used for extreme-scale computing, we have developed a scalable parallel data compression solution to reduce the size of large-scale data with low computational cost and minimal error. We use the proper orthogonal decomposition (POD) method to compress data because this method can effectively extract the main features from the data, and the resulting compressed data can be linearly decompressed. Our implementation achieves high parallel efficiency with a binary load-distributed approach (as shown in Figure 3), which is similar to the binary-swap image composition method. This approach allows us to effectively use all of the processing nodes and to reduce the interprocessor communication cost throughout the parallel compression calculations. The results of tests using the K computer indicate the superior performance of the proposed design and implementation.

3.3.2. 2-3-4 Combination for Parallel Compression on the K computer

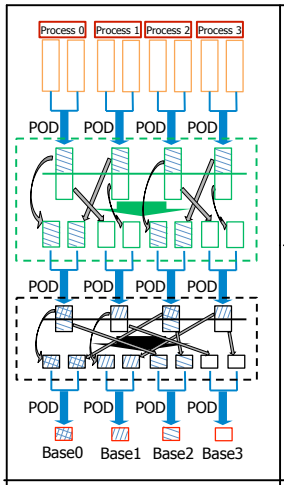


Figure 3 Parallel POD compression using our proposed binary load-distributed method.

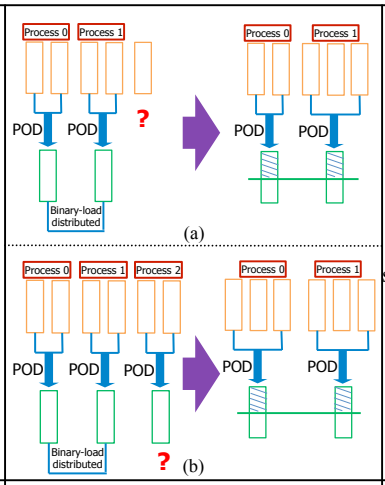


Figure 4 Two cases of non-power-of-two. (a) The number of time steps. (b) Both the number of the time steps and the processors.

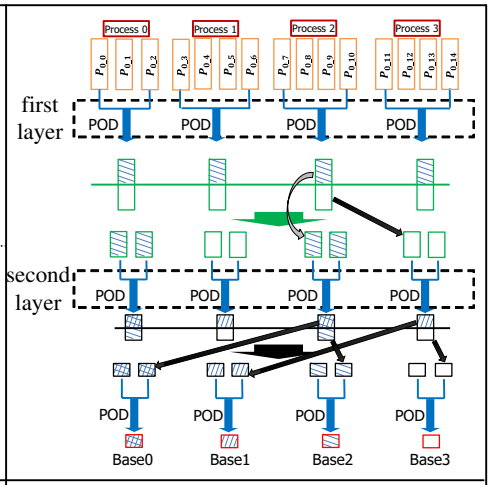


Figure 5 The data with 15 time steps are efficiently parallel compressed using our 2-3-4 combination approach. The best load balance was achieved.

In our previous research, a parallel compression method has been proposed. However, in this algorithm, interprocessor communication can only be carried out in the case that both the number of time steps and processors are power-of-two (the case in Figure 3). Obviously, it is

impossible for the general cases, Figure 4 shows two non-power-of-two cases. A method that can fully resolve this problem with low computational cost will be very popular. In this research, we proposed such an approach called 2-3-4 combination approach, which can be simply implemented and also reach high performance of parallel computing algorithms. Furthermore, our method can obtain the best balance among all parallel computing processors. This is achieved by transferring the non-power-of-two problem into power-of-two problem to fully use the best balance feature of the binary load-distributed method proposed in our first research. Figure 4 shows how to transfer the two non-power-of-two cases into power-of-two. Figure 5 is an example to effectively compress the data with 15 time steps through using our 2-3-4 combination method. We evaluate our approach through applying it to the parallel POD compression algorithm on the K computer.

3.4 A-Cell

An important mission of advanced visualization research team is to create reusable program modules that could be used by AICS and the rest of HPC community. Our projects include physics simulation and rendering. In addition we have lunched the new trend of knowledge discovery in simulation data. In order to make our solutions available for larger portion of the community our solutions should be completely portable and scalable to be more reusable. Therefore we decided to focus on the fundamental problem of portability and scalability. Other than the K computer, the visualization team uses a specific-purposed visualization cluster with heterogeneous nodes with two high-end CPUs and one GPU per node. It is desirable that our programs to be executable on both K computer and visualization cluster without modification or additional setup. Furthermore, it is desired that our programs to be executed without modification or additional setup on the next generation exa-scale supercomputer which its exact architecture is not currently determined yet.

Unfortunately, available solutions like OpenACC, OpenMP, PGAS, and Unified Memory in CUDA C only make the problem deeper. These technologies try to present the programmer with an abstraction of the system that looks and feels like a sequential programming environment. Then, the compiler will be responsible for creating a parallel program out of user code. However, most compilers fail to perform that task properly. In addition, compile-time parameters differ from one machine to another. That makes the program less portable. Furthermore, none of these technologies are portable between multi-core to many-core architectures and vice versa.

We came up with a promising solution that we call A-Cell (asynchronous cells). A-Cell is a high-level abstraction of fine-grained parallelism specifically designed to be applicable to all range of parallel devices from super computers based on CPUs or GPUs, to network of

embedded devices. To achieve this, A-Cell adopts a programming model called "connectionist computing" and with that takes a leap step farther from Turing programming model compared to aforementioned solutions. Also, in contrast with those other solutions that are based on holistic philosophy, the philosophy of A-Cell is reductionist. An A-Cell encapsulates a fine-grained task with its related variables and data linkage. A source-to-source compiler translates the program to a set of programs that are compilable to the target devices. Execution of the task is through massive instantiation of an A-Cell. The runtime environment takes the responsibility of distributing A-Cell instances between all available nodes, CPU cores or GPU multiprocessors (MPs). The runtime environment also assures synchronization and consistency of data between A-Cells.

With A-Cell two important inherent properties emerge, namely, Spatial Elasticity and Temporal Elasticity. Spatial Elasticity makes A-Cells to fit in any heterogeneous computing environment while Temporal Elasticity improves execution time by compensating for a part of interconnect latency and the time wasted by unexpected system interrupts. Development of A-Cell compiler based on LLVM/Clang compiler system has been started and it is about 20% through. A simulator is developed as a proof of concept for A-Cell scalability and its better time performance. The simulator is released to public and is available as an open-source project.

When the A-Cell compiler, runtime system becomes available, we will be able to produce visualization and knowledge discovery solutions that are portable between varieties of HPC environments and scalable to arbitrary number of nodes.

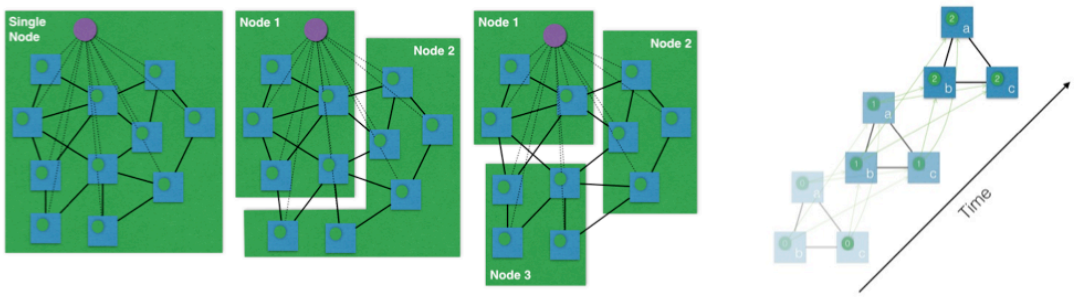


Figure 6. Left: Spatial Elasticity, Right: Temporal Elasticity in A-Cell.

4. Schedule and Future Plan

We will release our visualization software around mid. of FY2014, and have a plan to give lectures related our released software. Research themes and developed software will be investigated further in next year continuously, for instance, (1) Completion and release of

KnoRBA + A-Cell precompiler. KnoRBA is an original agent-based software development framework that can be used for development of a scalable, extensible and portable knowledge discovery solution, (2) Implementation of a demo user interface for wall-mounted display, and (3) To proceed with research and implementation of multi-modal knowledge discovery and data minding using KnoRBA and A-Cell.

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] Ono, K., Kawanabe, T., and Hatada, T., "HPC/PF - High Performance Computing Platform: An Environment That Accelerates Large-Scale Simulations, "Lecture Notes in Computer Science, Vol. 7851, pp. 23-27, 2013.

(2) Conference Papers

[2] Khandan, H., and Ono, K., "Knowledge Request-Broker Architecture: A Possible Foundation for A Resource-Constrained Dynamic and Autonomous Global Network", in *Proceedings of 2014 IEEE World Forum on Internet of Things*, ISBN 978-1-14799-3460-7, March 2014, Seoul, South Korea.

[3] Bi, C., and Ono, K., "2-3-4 Combination for Parallel Compression on the K Computer," in Proceedings of IEEE Pacific Visualization Symposium, pp. 281-285, March, 2014.

[4] Onishi, J. and Ono, K., "Development of a CFD software for large-scale computation," FLUCONME 2013, Nov. 18-23, 2013.

[5] Ono, K. and Mikami, K., "High-performance application development towards exa-scale computation" in Proceedings of 27th Computational Fluid Dynamics Symposium, Dec. 2013.

(3) Invited Talks

[6] Ono, K., "Strategy of Visualization toward Exascale Computing," PC cluster consortium workshop in Kyoto, Jan. 2013.

[7] Ono, K., "Life cycle management of big data for extreme-scale simulation," Big data and extreme-scale computing, Charleston, SC, USA, April, 2013.

[8] Ono, K., "Technology Infrastructure for Scientific Applications with Large-Scale Dataset," The 4th AICS International Symposium: Computer and Computational Science for Exascale Computing, Dec. 2013.

[9] Ono, K., "Challenge for parallel visualization of large-scale dataset and current status," Prospects for Massively Parallel Computing in Science and Technology Calculation - Use, Application and Problems, Tokyo Metropolitan University, March, 2014.

(4) Posters and Presentations

[10] Khandan, H., "Connectionism: How the World Really Computes", Oral and poster presentation at *11th Interdisciplinary Evening*, RIKEN Wako Campus, March 2014.

[11] Bi, C. and Ono, K., "Parallel POD Compression Accelerated by Binary-Swap Compositing," in Proceedings of Symposium on Advanced Computing Systems and Infrastructures 2013, pp. 112, May, 2013.

[12] Bi, C., Ono, K., Ma, K.-L., Wu, H., and Imamura, T., "Proper Orthogonal Decomposition Based Parallel Compression for Visualizing Big Data on the K Computer," in Proceedings of IEEE Symposium on Large-Scale Data Analysis and Visualization 2013, pp. 121-122, October, 2013.

[13] Bi, C. and Ono, K., "POD-Based Parallel Compression for Visualizing Large-Scale Dataset," Proceedings of High Performance Computing Symposium 2013, p.83, 2013.

(5) Patents and Deliverables

[14] CPMlib Cartesian Partitioning Manager library

[15] PMlib Performance Monitor library

[16] TextParser Parameter parsing library

[17] CIOlib Cartesian file I/O library

Data Assimilation Research Team

1. Team members

Takemasa Miyoshi (Team Leader)
Shigenori Otsuka (Postdoctoral Researcher)
Koji Terasaki (Postdoctoral Researcher)
Shunji Kotsuki (Postdoctoral Researcher)
Hazuki Arakida (Technical Staff)
Juan J. Ruiz (Visiting Scientist)
Shinichiro Shima (Visiting Scientist)
Masahiro Sawada (Visiting Scientist)
Shu-Chih Yang (Visiting Scientist)
Stephen G. Penny (Visiting Scientist)
Keiichi Kondo (Student Trainee)
Marimo Ohhigashi (Research Assistant)
Yukie Komori (Assistant)
Rie Deguchi (Assistant)

2. Research Activities

Data Assimilation Research Team (DA Team) was launched in October 2012 and is composed of 12 research and technical staff including 5 visiting members as of March 2014. Data assimilation is a cross-disciplinary science to synergize numerical simulations and observational data, using statistical methods and applied mathematics. As computers become more powerful and enable more precise simulations, it will become more important to compare the simulations with actual observations. DA Team performs cutting-edge research and development on advanced data assimilation methods and their wide applications, aiming to integrate computer simulations and observational data in the wisest way. Particularly, DA Team will tackle challenging problems of developing efficient and accurate data assimilation systems for high-dimensional simulations with large amount of data. The specific areas include 1) research on parallel-efficient algorithms for data assimilation with the super-parallel K computer, 2) research on data assimilation methods and applications by taking advantage of the world-leading K computer, and 3) development of most advanced data assimilation software optimized for the K computer.

In FY2013, we focused on data assimilation research in the following aspects: 1) theoretical research on challenging problems, 2) leading research on meteorological applications, 3) optimization of computational algorithms, and 4) exploratory research on wider applications.

We also explored close collaborations with several research teams within the AICS Research Division. We have made substantial progress on the following research items:

[Theoretical research]

1. A discrete Bayesian optimization approach to find optimal ensemble sizes in a multi-model ensemble Kalman filter (EnKF) was explored.
2. The approach to multi-scale covariance localization invented and investigated in FY2012 was further explored (2 papers published).
3. The role of observation error correlations in data assimilation was explored.
4. Potential impact of assimilation order of observations in serial EnKF was investigated.
5. Particle filter methods to treat non-Gaussian PDF were explored.

[Leading research on meteorological applications]

6. A Local Ensemble Transform Kalman Filter (LETKF) experiment with large ensemble up to 10240 members was performed to investigate the probability density function (PDF) of atmospheric flows more precisely. PDF plays an essential role in data assimilation.
7. The LETKF system with a global Nonhydrostatic ICosahedral Atmospheric Model (NICAM) was developed and tested with the real conventional observations, in collaboration with Computational Climate Science Research Team.
8. "Big Data Assimilation" to take advantage of Big Data from both high-resolution simulations and advanced sensors was explored. As a first step, next-generation phased array weather radar data were considered for assimilation.

[Computational optimization]

9. The high-performance eigenvalue solver "EigenExa" was applied to the LETKF in close collaboration with Large-scale Parallel Numerical Computing Technology Research Team.
10. The KMR (K Map Reduce) was applied to the LETKF workflow to maximize the efficiency with the K computer, in close collaboration with HPC Programming Framework Research Team.

[Wider applications]

11. A potential application of data assimilation to ecosystem simulations was explored.

Among the achievements, three achievements are selected and highlighted in the next section.

3. Research Results and Achievements

3.1. A discrete Bayesian optimization approach to multi-model EnKF

No simulation can be perfect, and data assimilation fills the gap between the imperfect simulations and real phenomena. Multi-model ensemble may account for uncertainties of simulation models, and previous studies in meteorological data assimilation showed advantage of multi-model ensemble Kalman filter (EnKF) in reducing the impact of the model errors.

In the previous studies, the ensemble sizes for each model are prescribed subjectively, for example, uniformly distributed to each model (Fig. 1 left). In this study, we adopt a Bayesian filter approach to a multi-model EnKF to find the optimal combination of ensemble sizes for each model (Fig. 1 right). We developed an effective inflation method to make the Bayesian filter work without converging to a single imperfect model.

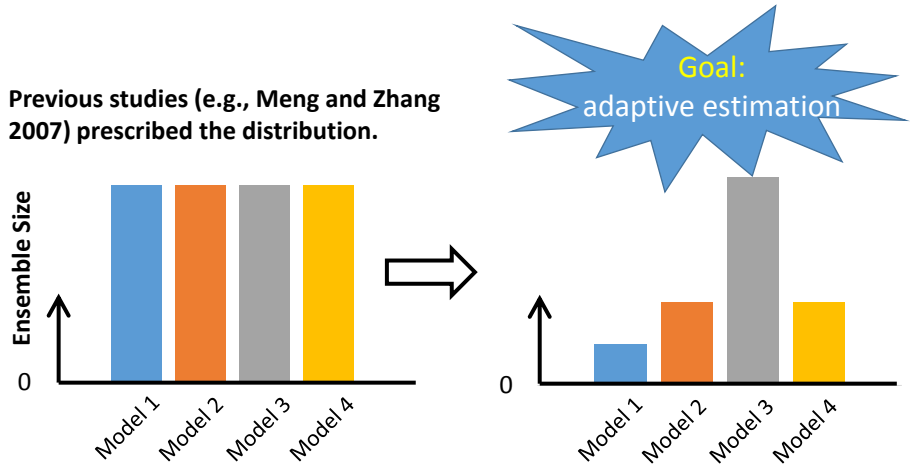


Figure 1. Schematic showing the motivation for the Bayesian optimization approach to multi-model EnKF. Four models (Model 1-4) are considered.

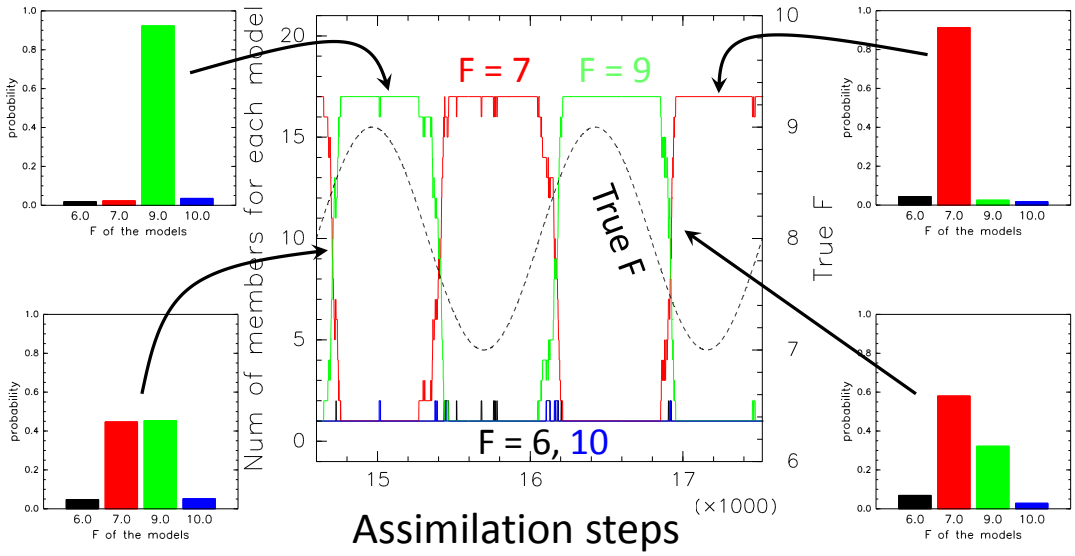


Figure 2. Results of the Bayesian optimization approach to multi-model EnKF. The largest center figure shows time series of true F (black dashed, right axis) and the estimated ensemble sizes (solid lines, left axis) for F=6 (black), 7 (red), 9 (green), and 10 (blue). The smaller four panels on both sides show the snapshot of PDF of each model at chosen instances (shown by arrows).

As a first step, we tested the proposed approach with the 40-variable Lorenz-96 model. Four different values of the model parameter F (F = 6, 7, 9, 10) were used to mimic the multi-model ensemble. When the true F had temporal variations $F = 8 + \sin(t)$, the proposed system followed the temporal change successfully (Fig. 2), and the RMSE was improved.

3.2. Multi-scale covariance localization

Following the theoretical development of the dual-localization approach in FY2012, in FY2013 a number of experiments were performed using an Atmospheric General Circulation Model (AGCM) with intermediate complexity known as the SPEEDY model, having led to two publications (Miyoshi and Kondo 2013; Kondo et al. 2013). The main findings are highlighted in this report.

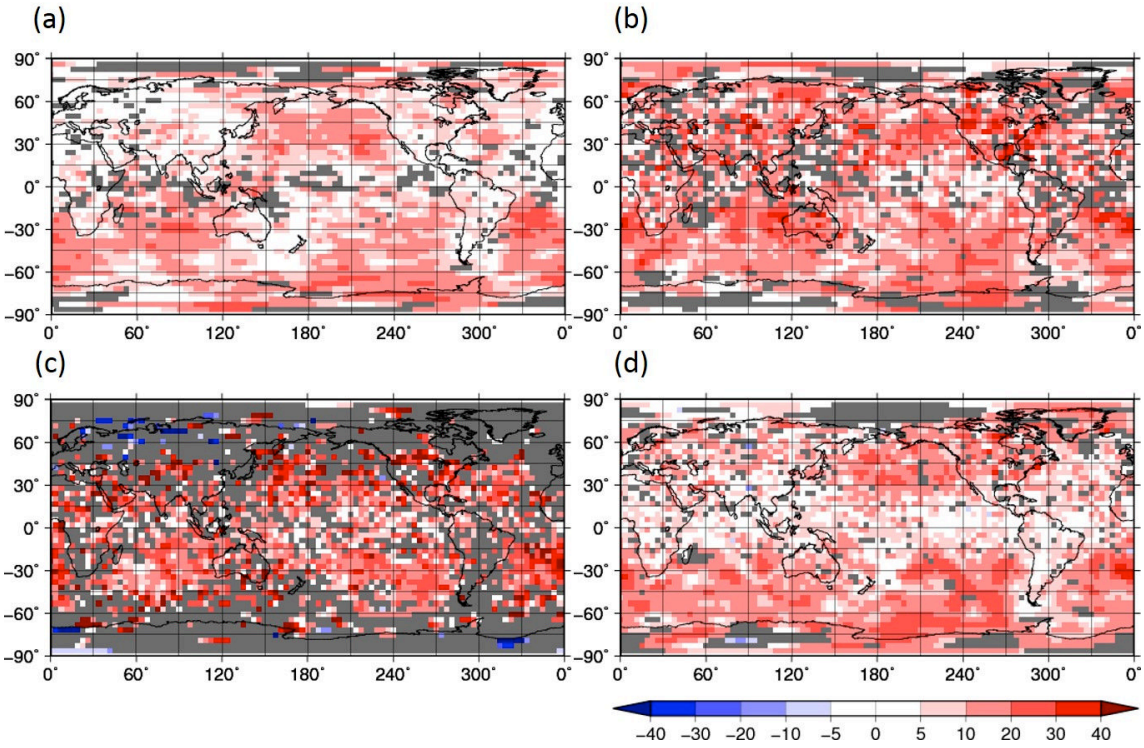


Figure 3. Improvements (%) of 1-year-average analysis RMSE of DLOC over CTRL for (a) zonal wind at the 4th model level (~500 hPa), (b) temperature (K) at the 2nd model level (~850 hPa), (c) specific humidity at the lowest level (~950 hPa), and (d) surface pressure. Red (blue) indicates advantage (disadvantage) of DLOC. Adapted from Fig. 6 of Miyoshi and Kondo (2013).

The newly proposed dual-localization method (DLOC) indicates astonishing improvements for all variables compared with the regular single localization (CTRL) (Fig. 3). DLOC uses two localization parameters, and the sensitivity to the two localization parameters is investigated. The results show that the dual-localization approach outperforms traditional single localization with relatively wide choices of the two localization scales by about 400-km ranges (Fig. 4). This

suggests that we could avoid fine tuning of the two localization parameters. We started adapting DLOC to a real typhoon case using the WRF-LETKF system and obtained improved representation of heavy rainfalls at meso-convective scales. Here, WRF stands for the Weather and Research Forecasting model, a widely-used community numerical weather prediction model.

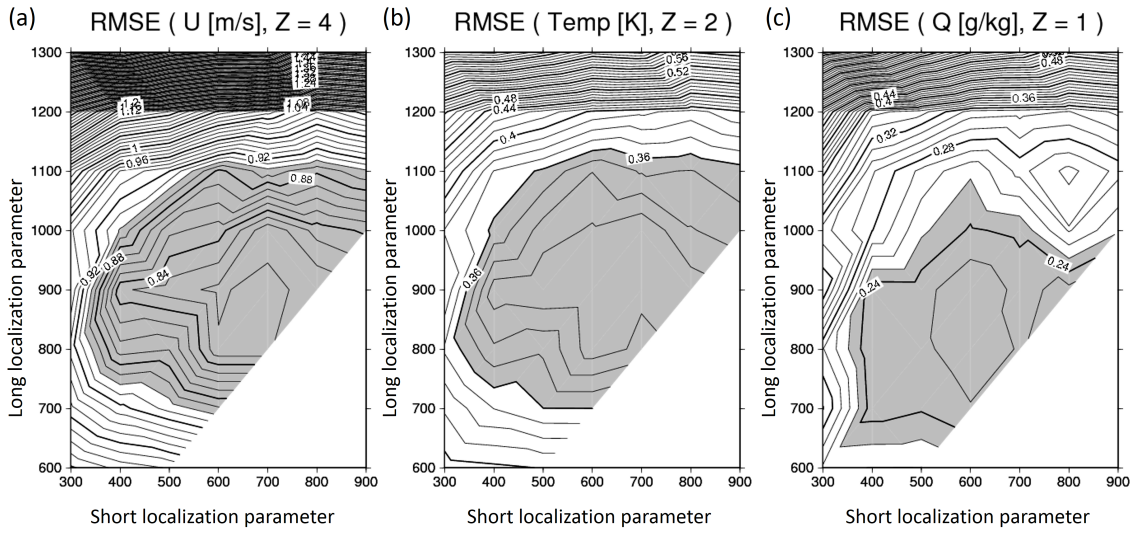


Figure 4. Analysis RMSEs of dual localization with various localization scale parameters, averaged for a year from 0000 UTC 1 February 1982 to 0000 UTC 1 February 1983 for (a) zonal wind (m s^{-1}) at the 4th model level, (b) temperature (K) at the second model level and (c) specific humidity (g kg^{-1}) at the lowest model level. The RMSEs of CTRL are 0.900 m s^{-1}, 0.366 K and 0.258 g kg^{-1}, respectively. The shaded areas indicate improvements of DLOC over CTRL. Adapted from Fig. 5 of Kondo et al. (2013).

3.3. Developing the NICAM-LETKF system

The local ensemble transform Kalman filter (LETKF) was applied to the Nonhydrostatic ICosahedral Atmospheric Model (NICAM). Taking advantage of the existing LETKF code for efficient development, our first version of the NICAM-LETKF prototype system (Fig. 5) has the LL-to-ICO grid conversion and its inverse, where LL and ICO represent Longitude-Latitude and ICOsahedral grid structures for the existing LETKF code and NICAM, respectively. Without making substantial changes to the existing codes, the grid conversions act as adapters between the existing NICAM and LETKF. With this prototype, we assimilated successfully the National Centers for Environmental Prediction (NCEP) PREPBUFR observational data, a dataset from the NCEP operational Global Data Assimilation System (GDAS) containing global conventional observations such as reports from surface stations, ships, ocean buoys, weather balloons and aircrafts, and satellite-based winds.

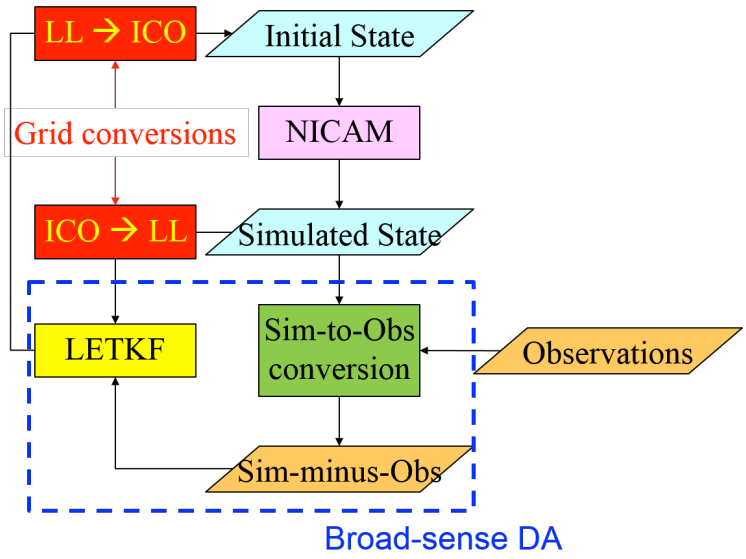


Figure 5. Flow-chart of the NICAM-LETKF prototype system.

After 5 days of data assimilation, the NICAM-LETKF produced the analysis with high correlation with other analysis data from operational numerical weather prediction centers (Fig. 6). This confirms the successful implementation of the NICAM-LETKF data assimilation system.

We also started making substantial changes to the LETKF interface, so that the LL-ICO grid conversions are no longer needed. This will reduce the significant I/O and interpolation errors due to the grid conversions. We developed a preliminary version of the NICAM-LETKF without LL-ICO conversions, and confirmed that the computer time was reduced by about 40% (Fig. 7).

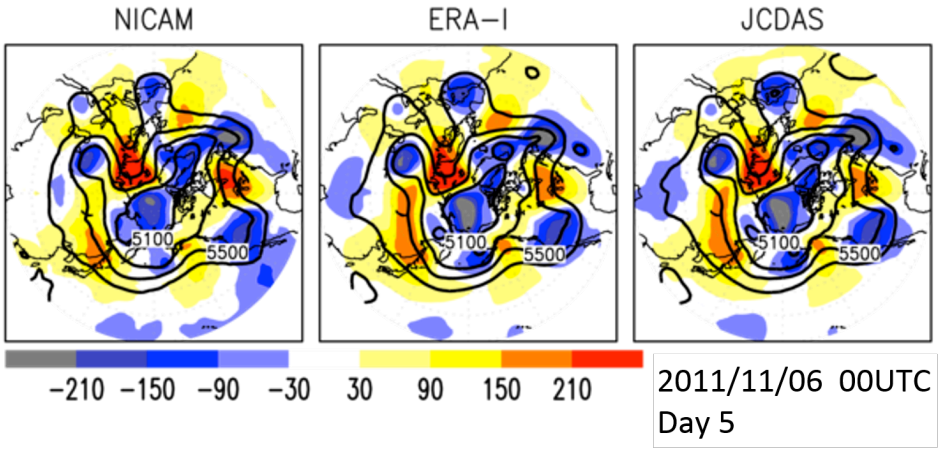


Figure 6. 500-hPa geopotential height analysis on 0000 UTC 6 November 2011 from the NICAM-LETKF (left, the 5th day of data assimilation), European Reanalysis ERA Interim (middle), and Japanese Climate Data Assimilation System (right).

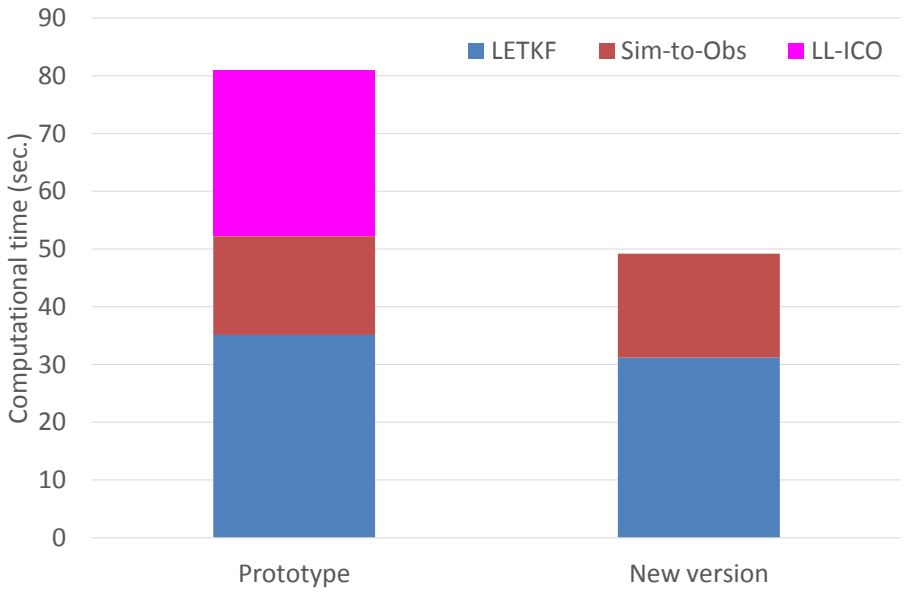


Figure 7. Computational time of the two versions of NICAM-LETKF at a G-level 6 (112 km) resolution using 200 nodes of the K computer. Left: prototype version with LL-ICO grid conversions, Right: new version without grid conversion.

3.4. Application of KMR (K Map Reduce) to LETKF workflow

The LETKF workflow had a large number of small jobs, and we applied KMR (K Map Reduce) to optimize the workflow. KMR is developed and maintained by HPC Programming Framework Research Team, and this work is a good example of interdisciplinary collaborations between computer science and computational science within AICS Research Division.

The WRF-LETKF system has *N* separate jobs for ensemble forecasting, where *N* is the ensemble size (Fig. 8). We have a single job for the LETKF. Here, we consider WRF-LETKF as an example, but the results and discussions can be generalized to any model. When *N* = 41, it took about 2 hours to complete the 41-member ensemble forecasts (Fig. 9). For robustness, we measured the timing 4 times and took the median. The median of the run time of the WRF forecast was about 2 minutes, and the submitted job had a size of 15 nodes for an hour. An hour may sound too long, but occasionally, it could take up to an hour, so we had to assign an hour to avoid unexpected failure. Due to the limit of the number of simultaneous job submissions in the K computer, we could submit either 15 or 20 jobs simultaneously. Therefore, we had almost 2 hours of the wait time to compete all 41 WRF forecasting jobs (Fig. 9).

This situation may be ameliorated by applying the KMR. "Map Reduce" fits very well with the LETKF workflow (Fig. 8), and can easily combine the *N* forecasting jobs into one. We applied the KMR and combined the 41 small jobs (15 nodes for an hour) into a single large job (630 nodes for

an hour). The total computational request is very similar (630 node-by-hour product), but the number of jobs is different (41 vs. 1). As a result, we could accelerate the total wall-clock time to be about 8 minutes (compared with 120 minutes!) (Fig. 10). For robustness, we measured the timing 9 times and took the median. What is different is the wait time. The K computer wait time in the queue turned out to be much smaller for 630 nodes for an hour, rather than submitting 15 or 20 jobs simultaneously for 15 nodes for an hour.

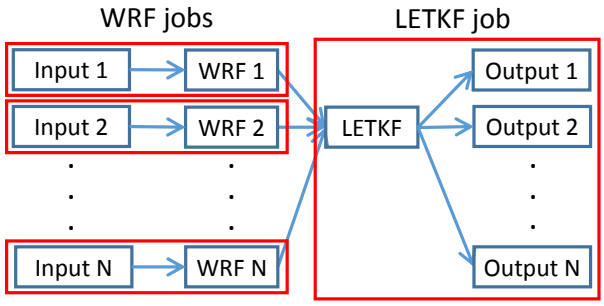


Figure 8. Schematic showing LETKF workflow. Blue and red boxes indicate each process and job, respectively. "Input" processes generate input data to the WRF forecast, "WRF" processes compute the forecast, "LETKF" process is data assimilation, and "Output" processes convert the file formats.

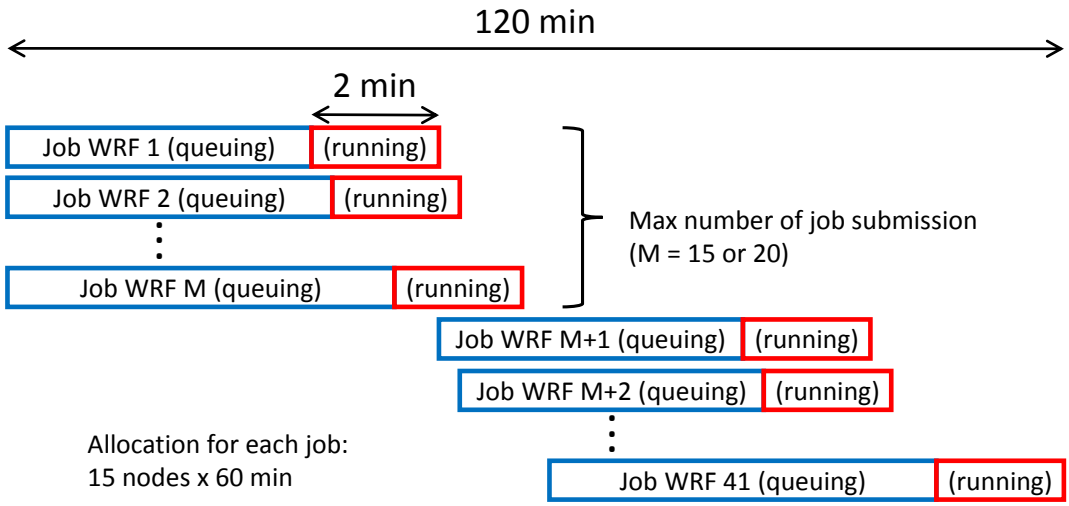


Figure 9. Wall-clock time for computations of the 41-member WRF ensemble forecasts.

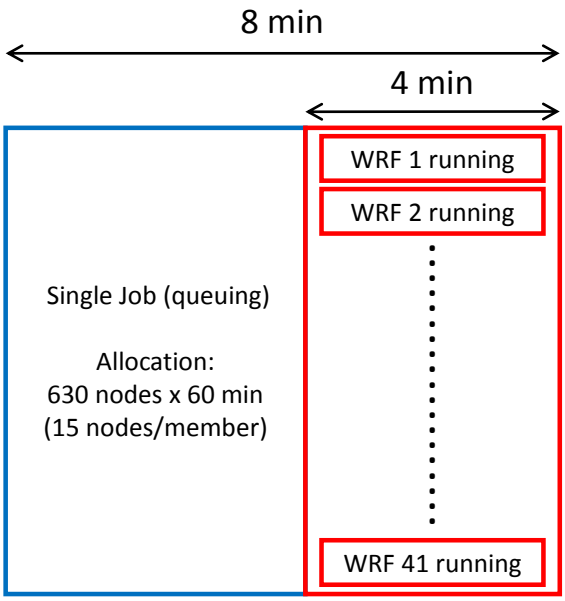


Figure 10. Wall-clock time for the same WRF ensemble forecasts as Fig. 9, but with KMR combining the 41 separate jobs into one.

4. Schedule and Future Plan

In FY2013, Team had three additional full-time research and technical staff and accepted visiting researchers, leading to a substantial growth. We started working on a wide range of data assimilation research on theoretical explorations, leading meteorological applications, algorithmic optimization, and wider applications. Our active research efforts started making impact on the scientific communities, and we are in a good shape in making progress on the research items of the AICS road-map. In FY2014, we will further extend and strengthen what we have achieved so far, and also will keep seeking new challenges. Making the most use of Big Data is an important emerging direction, and we are taking the lead in what we call the "Big Data Assimilation" concept. We will keep updating ourselves with the most recent movements and trends in the scientific community and society, while making substantial progress on traditional research.

Team will have a few more additional research staff in FY2014. Team is still young and spinning up, but will keep the consistent and competitive level of productivity, aiming to be one of the world's leaders in the field of data assimilation.

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] Onogi, K., Y. Harada, S. Kobayashi, H. Kamahori, C. Kobayashi, K. Endo, T. Ishibashi, M.

Kubota, K. Yoshimura, **T. Miyoshi**, N. Komori, and K. Oshima, 2012: Report on WCRP International Reanalysis Conference. *Tenki*, **59**, 1007-1016. (in Japanese)

[2] Kobayashi, K., **S. Otsuka**, K. Takara, S. Origuchi, and K. Saito, 2013: Ensemble prediction of heavy rainfalls and floods around small- to medium-size rivers. *Annual J. Hydraulic Engineering*, **57**, 1597-1602. (in Japanese)

[3] Yoshimura, K., **T. Miyoshi**, and M. Kanamitsu, 2013: Idealized experiments of water isotopes using an ensemble Kalman filter. *J. Japan Society of Civil Engineers B1 (Hydraulic Engineering)*, **69**, 1795-1800. (in Japanese)

[4] Iwasaki, T., K. Ito, H. Miura, **S. Otsuka**, Y. Baba, A. Hashimoto, K. Saito, T. Hara, A. Noda, and **M. Sawada**, 2013: Report on the Second International Workshop on Nonhydrostatic Numerical Models. *Tenki*, **60**, 209-215. (in Japanese)

[5] **Ruiz, J. J.**, M. Pulido, and **T. Miyoshi**, 2013: Estimating model parameters with ensemble-based data assimilation: A review. *J. Meteorol. Soc. Japan*, **91**, 79-99. doi:10.2151/jmsj.2013-201

[6] Enomoto, T., **T. Miyoshi**, Q. Moteki, J. Inoue, M. Hattori, A. Kuwano-Yoshida, N. Komori, and S. Yamane, 2013: Observing-system research and ensemble data assimilation at JAMSTEC. *Data Assimilation for Atmospheric, Oceanic and Hydrologic Applications (Vol. II)*, ed. by S. K. Park and L. Xu, chap. 21, 509-526, Springer, doi:10.1007/978-3-642-35088-7_21.

[7] Norwood, A., E. Kalnay, K. Ide, **S.-C.Yang**, and C. Wolfe, 2013: Lyapunov, singular and bred vectors in a multi-scale system: an empirical exploration of vectors related to instabilities. *Journal of Physics A, special issue of Lyapunov vectors*, **46**, 20.pp.1. doi:10.1088/1751-8113/46/25/254021

[8] Ushiyama, T., T. Sayama, S. Fujioka, Y. Tatebe, K. Fukami, and T. Miyoshi, 2013: Rain-runoff prediction experiments of 12th and 15th Typhoon in 2011 using ensemble Kalman filtering. *J. River Technology*, **18**, 319-324. (in Japanese)

[9] Lien, G.-Y., E. Kalnay, and **T. Miyoshi**, 2013: Effective Assimilation of Global Precipitation: Simulation Experiments. *Tellus*, **65A**, 11915. doi:10.3402/tellusa.v65i0.19915

[10] Arabas, S. and **S. Shima**, 2013: Large Eddy Simulations of Trade-Wind Cumuli using Particle-Based Microphysics with Monte-Carlo Coalescence. *J. Atmos. Sci.*, **70**, 2768-2777. doi: 10.1175/JAS-D-12-0295.1

[11] Ota, Y., J. C. Derber, E. Kalnay, and **T. Miyoshi**, 2013: Ensemble-based observation impact estimates using the NCEP GFS. *Tellus*, **65A**, 20038. doi:10.3402/tellusa.v65i0.20038

[12] **Ruiz, J. J.**, M. Pulido, and **T. Miyoshi**, 2013: Estimating model parameters with ensemble-based data assimilation: Parameter covariance treatment. *J. Meteorol. Soc. Japan*, **91**, 453-469. doi:10.2151/jmsj.2013-403

[13] **Miyoshi, T.**, **S. Otsuka**, N. Komori, T. Tsuyuki, T. Enomoto, 2013: Report on AICS International Workshop on Data Assimilation. *Tenki*, **60**, 731-735. (in Japanese)

[14] **Yang, S.-C.**, K.-J. Lin, **T. Miyoshi**, and E. Kalnay, 2013: Improving the spin-up of regional EnKF for typhoon assimilation and forecasting with Typhoon Sinlaku (2008). *Tellus*, **65A**, 20804. doi:10.3402/tellusa.v65i0.20804

[15] **Kondo, K.**, **T. Miyoshi** and H. L. Tanaka, 2013: Parameter sensitivities of the dual-localization approach in the local ensemble transform Kalman filter. *SOLA*, **9**, 174-177. doi:10.2151/sola.2013-039

[16] **Penny, S. G.**, E. Kalnay, J. A. Carton, B. R. Hunt, K. Ide, **T. Miyoshi**, and G. A. Chepurin, 2013: The local ensemble transform Kalman filter and the running-in-place algorithm applied to a global ocean general circulation model. *Nonlin. Processes Geophys.*, **20**, 1031-1046. doi:10.5194/npg-20-1031-2013

[17] **Miyoshi, T**. and **K. Kondo**, 2013: A multi-scale localization approach to an ensemble Kalman filter. *SOLA*, **9**, 170-173. doi:10.2151/sola.2013-038

[18] **Kotsuki, S.**, K. Tanaka., and S. Watanabe, 2014: Projected hydrological changes and their consistency under future climate in the Chao Phraya River Basin using multi-model and multi-scenario of CMIP5 dataset. *Hydrological Research Letters*, **8**, 27-32. doi:10.3178/hrl.8.27

[19] Watanabe, S., Y. Hirabayashi., **S. Kotsuki.**, N. Hanasaki., K Tanaka., C.M.R. Mateo., M. Kiguchi., E. Ikoma., S. Kanae., T. Oki., 2014: Application of performance metrics to climate models for projecting future river discharge in the Chao Phraya River basin, *Hydrological Research Letters*, **8**, 33-38. doi:10.3178/hrl.8.33

[20] **Kotsuki, S.** and K. Tanaka, 2014: Improvement of global crop calendar product using satellite-sensed vegetation indexes. *J. Japan Society of Civil Engineers B1 (Hydraulic Engineering)*, **70**, 259-264. (in Japanese)

(2) Conference Papers

[21] **Kostuki, S.** and K. Tanaka, 2014: Comparison of soil moisture derived from AMSR-E and land surface model in West African arid regions. *Proceedings of the Soil Moisture Workshop 2013*, 33-36. (in Japanese)

(3) Invited Talks

[22] **Yang, S.-C.**, K.-J. Lin, **T. Miyoshi** and E. Kalnay: Improving the spin-up of the regional EnKF for typhoon assimilation and forecast. AICS International Workshop on Data Assimilation, RIKEN, Japan, Feb, 2013.

[23] **Yang, S.-C.**, S.-Y. Chen, S.-H. Chen, C.-Y. Huang and C.-S. Chen: Evaluating the impact of the COSMIC-RO bending angle data on predicting the heavy precipitation episode on 16 June 2008 during SoWMEX-IOP8. Seminar at Korea Institute of Atmospheric Prediction Systems, Korea, 19th Aug, 2013.

[24] **Otsuka, S.**, M. Takeshita, and S. Yoden: Numerical experiments on formation of tropopause

inversion layer associated with extratropical cyclone. WCRP regional workshop on stratosphere-troposphere processes and their role in climate, Kyoto, 2nd Apr, 2013.

[25] **Shima, S.**: Super-Droplet Approach to Simulate Precipitating Trade-Wind Cumuli - Comparison of Model Results with RICO Aircraft Observations. International Workshop on Numerical Simulations of Particle/Droplet/Bubble-laden Multiphase Flows, JAMSTEC Tokyo office, Japan, 24th May, 2013.

[26] **Miyoshi, T.**: Computational Challenges in Big Data Assimilation with Extreme-scale Simulations. Big Data and Extreme-Scale Computing (BDEC) Workshop, Charleston, SC, USA, 1st May, 2013.

[27] **Miyoshi, T.**: "Data Assimilation Research on Typhoons. Biannual Meeting of the Meteorological Society of Japan, Tokyo, Japan, May, 2013.

[28] **Miyoshi, T.**: Exploring multi-scale and model-error treatments in ensemble data assimilation. Davos Atmosphere and Cryosphere Assembly DACA-13, Davos, Switzerland, 9th July, 2013.

[29] **Miyoshi, T.**: "Special Lecture Numerical Weather Prediction Ⅰ/Ⅱ: Numerical Weather Prediction Chaos, Predictability, and Data Assimilation", "Lecture: Localization and Inflation techniques in ensemble data assimilation", Summer School/Creative Workshop on Data Assimilation & Inverse Problems, Reading, UK, 25th July, 2013.

[30] **Miyoshi, T.**: Exploring Multi-scale and Model-error Treatments in Ensemble Data Assimilation. Sixth WMO Symposium on Data Assimilation, College Park, MD, USA, 8th Oct, 2013.

[31] **Miyoshi, T.**: Advances and challenges in ensemble data assimilation. RIMS International Conference on Theoretical Aspects of Variability and Predictability of Weather and Climate Systems, Kyoto, Japan, 25th Oct, 2013.

[32] **Yang, S.-C.**: Improving severe weather prediction in Taiwan using an advanced regional data assimilation system, National Cheng-Jung University, Taiwan. November, 2013.

[33] **Miyoshi, T.**: IMA Hot Topics Workshop : Exploring Multi-scale and Model-error Treatments in Ensemble Data Assimilation. Predictability in Earth System Processes, IMA, University of Minnesota, Minneapolis, MN, USA, 18th November, 2013.

[34] **Miyoshi, T.**: Toward severe-weather forecasting through "Big Data Assimilation". Second International Symposium on Watercourse Sensing and Operational Monitoring, Kyoto, Japan, 27th Novemver, 2013.

[35] **Miyoshi, T.**: Predicting sudden severe rainstorm using observational data and simulations. 9th workshop on information technology for safe life, The Institute of Image Electronics Engineers of Japan, Tokyo, 31 January, 2014. (in Japanese)

[36] **Miyoshi, T.**: Exploring Multi-scale and Model-error Treatments in Ensemble Data Assimilation. International Symposium on Data Assimilation 2014, Munich, Germany, 26th Feb, 2014.

[37] **Miyoshi, T.**: Innovating "Big Data Assimilation" technology for revolutionizing very-short-range severe weather prediction. International movement of Big Data application, Tokyo, 4 March, 2014. (in Japanese)

[38] **Miyoshi, T.**: Predict Sudden Severe Rainstorm with Data Assimilation. TEDxSannomya, Kobe, 9 March 2014. (in Japanese)

[39] **Miyoshi, T.**: Big Data Assimilation. Workshop on Earth fluids data analysis and numerical computation, Kobe, 11 March 2014. (in Japanese)

[40] **Miyoshi, T.**: Ensemble Kalman Filter in Meteorology and "Big Data Assimilation". Mathematical Science on Big Data Assimilation in Meteorology, Kyoto, Japan, 19th Mar, 2014.

(4) Posters and Presentations (selected English presentations)

[41] **Yang, S.-C.**, S.-Y. Chen, S.-H. Chen, C.-Y. Huang and C.-S. Chen: Evaluating the impact of the COSMIC-RO bending angle data on predicting the heavy precipitation episode on 16 June 2008 during SoWMEX-IOP8, 93rd AMS Annual Meeting.

[42] **Yang, S.-C.**, K.-J. Lin, **T. Miyoshi** and E. Kalnay: Improving the spin-up of the regional EnKF for typhoon assimilation and forecast with the 2008 Typhoon Sinlaku, 93rd AMS Annual Meeting.

[43] **Yang, S.-C.**, S.-Y. Chen, S.-H. Chen, C.-Y. Huang and C.-S. Chen: Evaluating the impact of the COSMIC-RO bending angle data on predicting the heavy precipitation episode on 16 June 2008 during SoWMEX-IOP8, International conference for GPS Radio Occultation, Taiwan (English)

[44] **Otsuka, S.**, M. Takeshita, S. Yoden: Numerical Simulation on the Formation of Tropopause nversion Layer by Gravity Waves Associated with an Extratropical Cyclone. AOGS, Brisbane, AS07-D5-PM1-P7-004, 28th Jun, 2013.

[45] **Otsuka, S.**, M. Takeshita, S. Yoden: A Numerical Experiment on the Formation of Tropopause Inversion Layer by Gravity Waves Associated with an Extratropical Cyclone. Davos Atmosphere and Cryosphere Assembly 2013, Davos, #415, 11th Jul, 2013.

[46] **Otsuka, S.**, N.J. Trilaksono, S Yoden: Statistical Analysis on the Size Distributions of Tropical Convective Systems during the Jakarta Flood Event in 2007 Simulated by JMA-NHM. Davos Atmosphere and Cryosphere Assembly 2013, Davos, #417, 12th Jul, 2013.

[47] **Yang, S.-C.** and E. Kalnay: Application of Ensemble Sensitivity to Data Assimilation. 6th WMO data assimilation workshop, USA

[48] Dillon M.E., **J.J. Ruiz**, E.A. Collini, Y. Garcia-Skabar, E. Kalnay, **T. Miyoshi**, M. Kunii: Application of the WRF-LETKF system over Argentina: A Case Study. Sixth WMO Symposium on Data Assimilation, College Park, MD, USA, 8th Oct, 2013.

[49] Chang, C.-C., **S.-C. Yang** and C. Keppenne: Applications of the mean re-recentering scheme

to improve typhoon track prediction: A case study of typhoon Nanmadol (2011). 2013 APEC Typhoon Symposium, Taiwan.

[50] Tsai, C.-C., **S.-C. Yang**, and Y.-C. Liou, 2013b: Improving Short-Term QPFs with a WRF-LETKF Radar Data assimilation system: real case study with Typhoon Morakot. 2013 APEC Typhoon Symposium, Taiwan.

[51] Chang, C.-C., **S.-C. Yang** and C. Keppenne, 2013: Applications of the mean re-recentering scheme to improve typhoon track prediction: A case study of typhoon Nanmadol (2011). RIMS International Conference on Theoretical Aspects of Variability and Predictability in Weather and Climate Systems, Kyoto, 23rd Oct, 2013.

[52] **Yang, S.-C.**, E. Kalnay and E. Enomoto: Application of Ensemble Sensitivity to Data Assimilation, RIMS International Conference on Theoretical Aspects of Variability and Predictability in Weather and Climate Systems, Kyoto, 23rd Oct, 2013.

[53] **Otsuka, S.** and **T. Miyoshi**: A Bayesian optimization approach to multi-model ensemble data assimilation. RIMS International Conference on Theoretical Aspects of Variability and Predictability in Weather and Climate Systems, Kyoto, 22nd Oct, 2013.

[54] **Kondo, K.** and **T. Miyoshi**: Parameter sensitivities of the dual-localization approach in the SPEEDY-LETKF. RIMS International Conference on Theoretical Aspects of Variability and Predictability in Weather and Climate Systems, Kyoto, 25 Oct, 2013.

[55] **Otsuka, S.**, N. J. Trilaksono, and S. Yoden: Statistics on Convective Systems during the Jakarta Flood Event in 2007 Simulated byJMA-NHM. GCOE-ARS Final Symposium 2013, Uji, S2-7, 1st Dec, 2013.

[56] **Kondo, K.**, **T. Miyoshi**, H. L. Tanaka: Parameter sensitivities of the dual-localization approach in the SPEEDY-LETKF. The 4th AICS International Symposium, Kobe, 2nd Dec, 2013.

[57] **Terasaki, K.** and **T. Miyoshi**: Data Assimilation with error-correlated observations. The 4th AICS International Symposium, Kobe, 2nd Dec, 2013.

[58] **Otsuka, S.** and **T. Miyoshi**: A Bayesian optimization approach to multi-model ensemble data assimilation. The 4th AICS International Symposium, Kobe, 2nd Dec, 2013.

[59] **Kotsuki, S.** and K. Tanaka: Estimating impacts on terrestrial water cycle by integrating reservoir operation and irrigation processes to hydrological simulation. AMS 94th Annual Meeting, Atlanta, Georgia, 4th Feb, 2014.

[60] **Otsuka, S.** and **T. Miyoshi**: Bayesian optimization of multi-model ensemble data assimilation for a low-order model. AMS 94th Annual Meeting, Atlanta, Georgia, 6th Feb, 2014.

[61] **Arakida, H.**, **T. Miyoshi**, T. Ise: A comparison between observed and simulated Leaf Area Index toward data assimilation with a dynamical global vegetation model. Mathematical Science on Big Data Assimilation in Meteorology, Kyoto, 20th Mar, 2014.

[62] **Kotsuki, S.**, **S. Otsuka**, **T. Miyoshi** and Greybush S: Does assimilation order of Serial EnSRF affect analysis accuracy? : Idealized simulation with Lorenz-96. Mathematical Science on Big

Data Assimilation in Meteorology, Kyoto, 20th Mar, 2014.

[63] **Otsuka, S.** and **T. Miyoshi**: A Bayesian optimization approach to multi-model ensemble Kalman filter. Mathematical Science on Big Data Assimilation in Meteorology, Kyoto, 20th Mar, 2014.

[64] **Kondo, K.**, **T. Miyoshi** and H. L. Tanaka: The dual-localization approach and large ensemble data assimilation. Mathematical Science on Big Data Assimilation in Meteorology, Kyoto, 20th March, 2014.

[65] **Terasaki, K.**, **M. Sawada.**, and **T. Miyoshi**: Developing the Local Ensemble Transform Kalman Filter with the Japanese Icosahedral Global Model NICAM. Mathematical Science on Big Data Assimilation in Meteorology, Kyoto, 20th Mar, 2014.

(5) Patents and Deliverables

[66] The LETKF code is updated as needed and available at https://code.google.com/p/miyoshi/.

Computational Chemistry Research Unit

1. Unit members

Kimihiko Hirao (Unit Leader)

Jong-Won Song (Research Scientist)

Yukio Kawashima (Research Scientist)

Takao Tsuneda (Senior Visiting Scientist)

Ram Kinkar Roy (Senior Visiting Scientist)

Rahul Kar (Visiting Scientist)

2. Research Activities

Electronic structure calculations are now indispensable not only for theoretical chemists, but also for experimental chemists to understand chemical phenomenon. Density functional theory (DFT) is a major tool to tackle chemical phenomenon theoretically. DFT efficiently calculate electronic structure with high accuracy, and its algorithm is suitable for parallel computing. DFT now plays an important role in applications of molecular science running on the K Computer. However, conventional DFT could not describe important properties such as van der Waals interaction and optical property, such as non-linear optics and charge-transfer excitation, which are essential for accurate calculations for large scaled molecular systems.

We have developed long-range corrected density functional theory (LC-DFT), which overcomes the drawbacks of conventional DFT mentioned above. Recently, we found that LC-DFT obtains accurate energies of highest occupied molecular orbital (HOMO) and lowest occupied molecular orbital (HOMO). The development of LC-DFT had a large impact in theoretical chemistry and the number of research based on LC-DFT is growing intensively. However, LC-DFT has yet difficulty in describing photochemical reactions. Photochemical process includes avoided crossing among electronic states, spin-forbidden transitions, and state transitions between high and low spins. These properties cannot be calculated accurately by LC-DFT so far.

The objective of our project is to establish LC-DFT to be a standard electronic structure theory by expanding its capability. We feature new developments of photo- and electro-chemical reaction theories and its high-speed computational algorithms for next-generation supercomputer “K”, and the elucidations of significant reaction mechanisms and the designs of new functional materials in photo and electrochemistry. We also aim to increase reliability of electronic structure calculation by improving the accuracy of LC-DFT.

3. Research Results and Achievements

3.1. Singularity-free hybrid functional with a Gaussian attenuating exact-exchange (Gau-PBE) in a plane-wave basis

Integrable singularity in the exact exchange calculations for hybrid density functionals, is an old and well-known problem in plane-wave basis widely used for electronic structure calculation of solid-state systems. We need to overcome this problem for accurate calculation of materials, because DFT using plane-wave basis is one of the major tools to tackle them. Recently, we developed a hybrid functional named Gau-PBE, which uses a Gaussian function as a modified Coulomb potential for the exact exchange in Gaussain-type-orbital software mainly used for electronic structure calculation of isolated molecules. We have further developed methods and efficient program for electronic structure calculation of solid-state systems. Our new method is

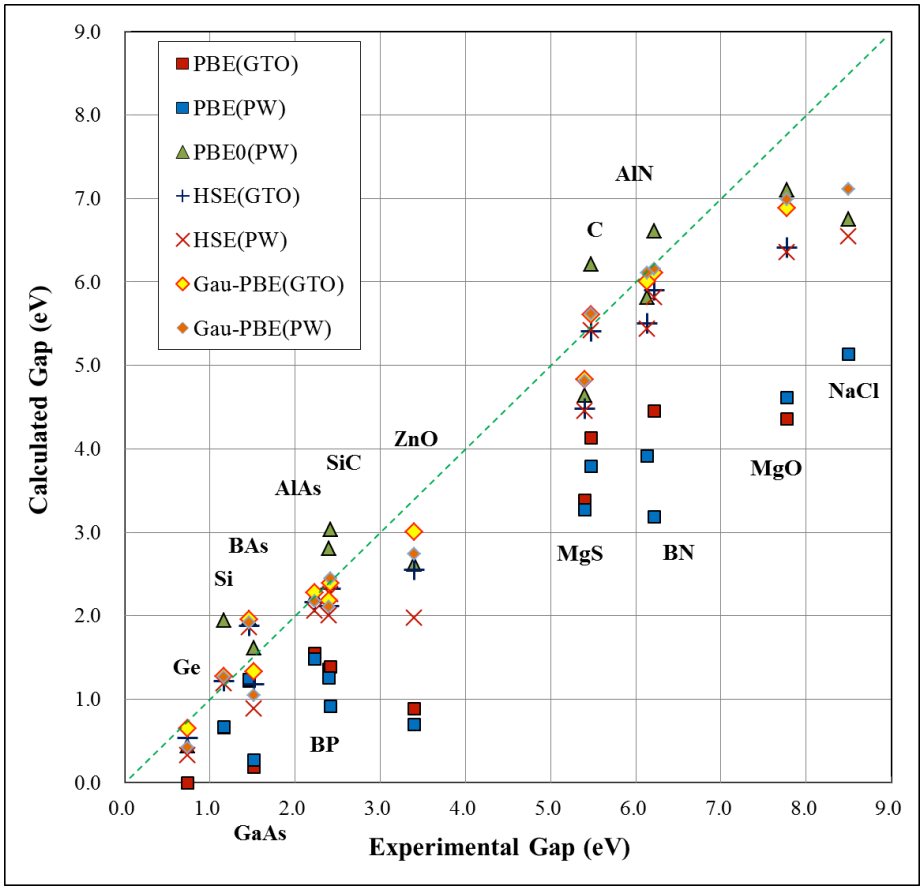


Figure 1. Calculated bandgap vs observed gap (Taken from J.-W. Song, G. Giorgi, K.Yamashita, K. Hirao, J. Chem. Phys., 138, 241101 (2013)).

implemented in a plane-wave-based software, Quantum ESPRESSO, widely used for electronic structure calculation of materials. We found the modified Coulomb potential of Gaussian function enables the exact exchange calculation in plane-wave basis to be singularity-free and, as a result, the Gau-PBE functional shows faster energy convergence on k and q grids for the

exact exchange calculations. Also, a tight comparison (same k and q meshes) between Gau-PBE, and two other well-known hybrid functionals, i.e. PBE0 and HSE06, indicates our new implemented functional as the least computational time consuming method (Figure 1). The Gau-PBE functional employed in conjunction with a plane wave basis provides bandgaps, an important property for material development, with higher accuracy than the PBE0 and HSE06 in agreement with bandgaps accurately calculated using Gaussian-type-orbitals. We found our new method promising for calculation of solid-state systems.

3.2. Long-range corrected density functionals combined with local response dispersion

Density functional theory, in general, underestimates the weak van der Waals type of intermolecular interactions. This is crucial in electronic structure calculation for large-sized molecular systems, which include the above weak interaction. We optimized parameters of the local response dispersion (LRD) method applied to the long-range corrected exchange-correlation functionals (LC-BOP12+LRD and LCgau-BOP+LRD) on the interaction energy for the complexes in the recently compiled S66 database. The new parameter optimization leads to highly accurate calculation for large systems. We found that calculation using our new parameter is comparable with the computationally demanding high-level wavefunction-based methods reported in Řezáč *et al.* (J. Chem. Theory Comput. 2011, 7, 2427). Our calculations with the S66 intermolecular complexes at equilibrium geometries suggest that LC-BOP12+LRD and LCgau-BOP+LRD are well-balanced and lower cost alternatives to the methods reported in the database. Further, critical test using the S66X8 database (with eight nonequilibrium points) and the HBC6 and NBC10 database shows LC+LRD method with newly optimized parameters is a promising candidate for dealing large molecular systems with such weak interactions.

3.3. Analysis of difference between intra- and inter-molecular charge transfer excitations in long-chained polyene

Charge transfer excitation plays an important role in various photochemical processes. It is still a challenge to describe charge transfer excitation for large-scaled molecular systems. For critical analysis of the performance of electronic structure calculation on charge transfer excitation, we performed intra- and inter-molecular charge transfer (CT) excitation calculations of $H_2N–(CH=CH)_n–NO_2$ (a) and its equidistant $[H_2N–H\cdots H–NO_2]$ complex (b) using EOM-CCSD (n=1–9), time-dependent (TD) LC-DFT (n=1–10). It was shown that LC-BOP and LCgau-BOP outperform all the tested DFT functionals on inter- and intra-CT excitation energy and oscillator strength, regardless of CT interaction distance (R). Decomposition of TD-DFT optical excitation energies of (a) and (b) into HOMO–LUMO gap and excitonic binding energy disclosed that HOMO–LUMO gap reduction resulting from delocalization of HOMO and LUMO through

bridged polyene conjugation is mainly responsible for the decreasing of intra-molecular CT excitation energy with polyene chain length, while inter-molecular CT increases linearly with –1/R, which is wholly due to the decrease in excitonic energy between HOMO and LUMO (Figure 2). The analysis provided wide understanding of charge transfer excitation and clues for further improvement of charge transfer excitation calculation. We found that success of exchange correlation functional on long-distanced intra-molecular CT calculations depends on correct descriptions of (1) Koopmans' energy of donor and acceptor and (2) excitonic energy between donor and acceptor, and (3) correct far-nucleus asymptotic behavior, –1/R. We found that LC scheme can satisfy (3), but needs an appropriate choice of long-range parameter able to satisfy (1) and (2). On the other hand, the pure, conventional hybrid, and screened hybrid functionals show near-zero intra- and inter-molecular excitonic energy regardless of R, which means optical band gap coincide with HOMO–LUMO gap. Therefore, we conclude that 100 % long-range Hartree–Fock exchange inclusion is indispensable for correct descriptions of intra-molecular CT excitations as well as inter-molecular CT. Our results indicate that bandgap calculation using conventional hybrids and screened hybrid functionals need reconsideration.

Figure 2. LUMO of $H_2N–(CH=CH)_{10}–NO_2$ obtained by LC-BOP (Taken from J.-W. Song, K. Hirao, Theor. Chem. Acc. 133, 1438(1-9) (2014)).

3.4. Path integral molecular dynamics simulation of hydrogen maleate anion based on range separated density functional theory

Ab initio path integral molecular dynamics (PIMD) simulation based on range separated DFT was performed to understand the nuclear quantum effect on the out-of-plane ring deformation of hydrogen maleate anion (Figure 3) and investigate the existence of a stable structure with ring deformation, which was suggested in experimental observation (Fillaux *et al.*, Chem. Phys. 1999, 120,

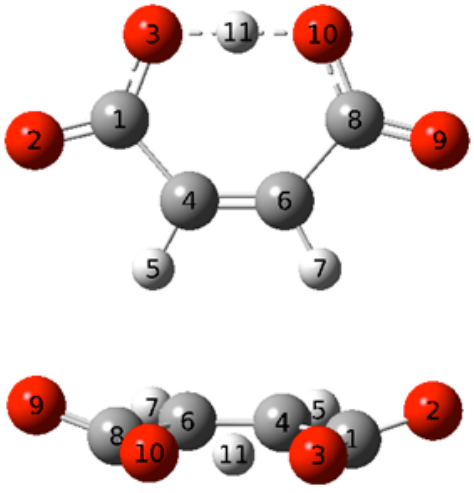


Figure 3. Hydrogen malonate anion and its ring-deformed structure.

387–403). The isotope effect and the temperature effect are studied as well. In our preliminary static calculation, we found that range separated DFT outperforms MP2 and conventional hybrid DFT. Thus, range separated DFT was used for our PIMD simulation. We first investigated the nuclear quantum effect on the proton transfer. In static calculation and classical *ab initio* molecular dynamics simulations, the proton in the hydrogen bond is localized to either oxygen atom. On the other hand, the proton is located at the center of two oxygen atoms in quantum *ab initio* PIMD simulations. The nuclear quantum effect washes out the barrier of proton transfer. We next examined the nuclear quantum effect on the motion of hydrogen maleate anion. Principal component analysis revealed that the out-of-plane ring bending modes have dominant contribution to the entire molecular motion. In quantum *ab initio* PIMD simulations, structures with ring deformation were the global minimum for the deuterated isotope at 300 K. We analyzed the out-of-plane ring-bending mode further and found that there are three minima along a ring distortion mode. We successfully found a stable structure with ring deformation of hydrogen maleate for the first time, to our knowledge, using theoretical calculation. The structures with ring deformation found in quantum simulation of the deuterated isotope allowed the proton transfer to occur more frequently than the planar structure. Static ab initio electronic structure calculation found that the structures with ring deformation have very small proton transfer barrier compared to the planar structure. We suggest that the "proton transfer driven" mechanism is the origin of stabilization for the structure with out-of-plane ring deformation.

4. Schedule and Research Plans

In the next fiscal year, we will continue our effort to expand the capabilities of LC-DFT. We will develop the order-*N* calculation algorithm of LC-DFT to calculate large molecular systems quantitatively with much less computational time. We will then apply this algorithm to excited state calculations on time-dependent density functional theory (TDDFT). We will also develop open-shell spin-orbit TDDFT to calculate molecular systems including metal atoms. Furthermore, we will develop a new method to calculate the nonadiabatic coupling among different electronic states, and carry out nonadiabatic coupling calculations based on TDDFT to reproduce photochemical reactions comprehensively. We are also planning to apply Gau-PBE and Gau-PBEh methods to solid-state calculations of real systems. We also aim to extend our TD-DFT based on LC-DFT to solid-state calculations as well.

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] "Self-interaction correction in density functional theory" T.Tsuneda, K.Hirao, J.

Chem. Phys., 140, 18A513 (1-13) (2014).

[2] "Accurate Prediction of Hyperfine Coupling Constant in Muoniated and Hydrogenated Ethyl Radicals: Ab Initio Path Integral Simulation Study with Density Functional Theory Method", K. Yamada, Y. Kawashima, M. Tachikawa, J. Chem. Theory. Comput., DOI: 10.1021/ct500027z

[3] "What makes differences between intra- and inter-molecular charge transfer excitations of conjugated long-chained polyene?: EOM-CCSD and LC-BOP study" J.-W. Song, K. Hirao, Theor. Chem. Acc. 133, 1438(1-9) (2014).

[4] "An *Ab Initio* Path Integral Molecular Dynamics Study of the Nuclear Quantum Effect on Out-of-plane Ring Deformation of Hydrogen" Y. Kawashima, M. Tachikawa, J. Chem. Theory Comp., 10, 153-163 (2014).

[5] "Long-range correction for density functional theory", T. Tsuneda, K. Hirao, Wiley Interdisciplinary Reviews: Computational Molecular Science, DOI: 10.1002/wcms.1178.

[6] "Communication: Singularity-free hybrid functional with a Gaussian attenuating exact-exchange (Gau-PBE) in a plane-wave basis" J.-W. Song, G. Giorgi, K. Yamashita, K. Hirao, J. Chem. Phys., **138**, 241101 (1-4) (2013).

[7] "Three-dimensional Reference Interaction Site Model Self-consistent Field Study of the Solvation and Electronic Structures of $[Cr(H_2O)_6]^{3+}$ in Aqueous Solution" S. Fujishige, Y. Kawashima, N. Yoshida, H. Nakano, J. Phys. Chem. A, 117, 8314-8322 (2013).

[8] "Long-range corrected density functionals combined with local response dispersion: A promising method for weak interactions", R. Kar, J.-W. Song, T. Sato, K. Hirao, J. Comput. Chem., 34, 2353-2359 (2013).

[9] "Stochastic Search of Molecular Cluster Interaction Energy Surfaces with Coupled Cluster Quality Prediction. The Phenylacetylene Dimer", M. A. Addicoat, Y. Nishimura, T. Sato, T. Tsuneda, S. Irle, J. Chem. Theory Comput., 9, 3848-3854 (2013).

(2) Books

[10] "Density Functional Theory in Quantum Chemistry" T. Tsuneda, Springer (2014).

(3) Invited Talks

[11] "Recent Advances in LC-DFT", K. Hirao, 4th AICS International Symposium, Kobe, December 2-3 (2013).

[12] "Recent Advances in LC-DFT", K. Hirao, The 8th General Meeting of ACCMS-VO (Asian Consortium on Computational Materials Science – Virtual Organization), Sendai, November 7th (2013).

[13] "Density functional theory for comprehensive orbital energy calculations", T. Tsuneda, 2013 International Workshop on Computational Science and Engineering, National Taiwan University, Oct. 14-17 (2013).

[14] "The K Computer and Recent Advances in DFT", K. Hirao, 2013 International Workshop on Computational Science and Engineering, National Taiwan University, Oct. 14-17 (2013).

[15] "DFT Exchange-Correlation Functionals and Correction", T. Tsuneda, JACI Computational Chemistry Lectures, JACI, Tokyo, Sep. 13 (2013). (In Japanese)

[16] "A Novel Analysis for Chemical Reaction Based on Orbital energies", T. Tsuneda, Special Symposium in The 62th Annual Meeting of The Japan Society for Analytical Chemistry, Kinki University, Osaka, Sep. 10th (2013). (In Japanese)

[17] "New World of Quantum Chemistry Lead by Long-Range Corrected Density Functional Theory", T. Tsuneda, 18th Lecture for Research Group on Computational Polymer Science, Tokyo Institute of Technology, Aug. 7th (2013). (In Japanese)

(4) Posters and Presentations

[18] "Configuration Search of Water Hexamer Anion: A Simulated Annealing Study", Y. Kawashima, H. Nakano, T. Sato, K. Yagi, "Dynamical ordering and integrated functions" 2nd International Symposium, Campus Plaza Kyoto, Kyoto, Jan. 11-12 (2014). (Poster)

[19] "The ring deformation of hydrogen maleate anion: A path integral molecular dynamics study", Y. Kawashima, M. Tachikawa, 5th International Symposium on Theoretical Chemistry, Todai-ji National Center, Nara, Dec. 2-6, (2013). (Poster)

[20] "Nuclear quantum effect on $OH^-(H_2O)_2$ with *ab initio* path integral molecular dynamics", Y. Ogata, Y. Kawashima. K. Takahashi, M. Tachikawa, 3rd International Conference on Molecular Simulation, Kobe International Conference Center, Kobe, Nov. 18-20 (2013). (Poster)

[21]"Quantum simulation for exotic molecules: Quantum Monte Carlo and Path Integral approac h", K. Koyanagi, Y. Kita, K. Yamada, Y. Kawashima, M. Tachikawa, 3rd International Conference on Molecular Simulation, Kobe International Conference Center, Kobe, Nov. 18-20 (2013). (Poster)

[22] "Singularity-free hybrid functional with a Gaussian attenuating exact-exchange (Gau-PBE) in a plane-wave basis"ingularity G. Giacomo, K. Yamashita, K. Hirao, Sixth Asia-Pacific Conference of Theoretical and Computational Chemistry, Gyeongju Hilton Hotel, Gyeongju, Jul. 10-13 (2013). (Poster)

[23] "The ring deformation of hydrogen maleate anion: A path integral molecular dynamics study", Y. Kawashima, M. Tachikawa, Sixth Asia-Pacific Conference of Theoretical and Computational Chemistry, Gyeongju Hilton Hotel, Gyeongju, Jul. 10-13 (2013). (Poster)

[24] "Theoretical investigation on the molecular and electronic structures of $Ti(Pc)_2$ and $Ti(Pc)_2^+$", M. Sumimoto, Y. Kawashima, K. Hori, H. Fujimoto, The 7th Annual Meeting of Japanese Society for Molecular Science, Kyoto TERRSA, Kyoto, Sep. 24-27 (2013). (Poster in Japanese)

[25] "*ab initio* path integral molecular dynamics study on the intramolecular hydrogen bond of hydrogen maleate", Y. Kawashima, M. Tachikawa, The 7th Annual Meeting of Japanese Society for Molecular Science, Kyoto TERRSA, Kyoto, Sep. 24-27 (2013). (Poster in Japanese)

[26] "Nuclear quantum effect on $OH^-(H_2O)_2$ with ab initio path integral molecular dynamics", Y. Ogata, Y. Kawashima, K. Takahashi, M. Tachikawa, The 7th Annual Meeting of Japanese Society for Molecular Science, Kyoto TERRSA, Kyoto, Sep. 24-27 (2013). (Poster in Japanese)

[27] "A LC-DFT + vdW Study of the Diels-Alder Reactions and the Global Hardness Response Analysis", R. K. Singh, T. Tsuneda, The 7th Annual Meeting of Japanese Society for Molecular Science, Kyoto TERRSA, Kyoto, Sep. 24-27 (2013).

[28] "Chemical reaction path analysis based on orbital energies", T. Tsuneda, The 7th Annual Meeting of Japanese Society for Molecular Science, Kyoto TERRSA, Kyoto, Sep. 24-27 (2013). (In Japanese)

[29] "A New Theory for Quantitative Description of Core and Valence Orbital Energies", A. Nakata, T. Tsuneda, 15th Annual Meeting of Theoretical Chemistry, May 15-17 (2013). (in Japanese)

[30] "Theoretical Chemistry for Exotic Molecular Systems", K. Koyanagi, Y. Kita, K. Yamada, Y. Kawashima, M. Tachikawa, 15th Annual Meeting of Theoretical Chemistry, May 15-17 (2013). (in Japanese)

[31] "ab initio Path Integral Molecular Dynamics Simulation for Analysis on Low-Barrier Hydrogen Bond of Protonated Lysine", Y. Ogata, M. Daido, Y. Kawashima, M. Tachikawa, 15th Annual Meeting of Theoretical Chemistry, May 15-17 (2013). (Poster in Japanese)

(5) Patents and Deliverables

[32] Song *et al.* implemented the newly developed theory "GauPBE" in an open source plane-wave-based quantum chemistry software: "Quantum ESPRESSO". http://www.quantum-espresso.org/

Computational Disaster Mitigation and Reduction Research Unit

1. Unit members

Muneo Hori (Unit Leader)

Hideyuki O-tani (Postdoctoral Researcher)

Jian Chen (Postdoctoral Researcher)

2. Research Activities

Computational disaster mitigation and reduction research unit is aimed at developing advanced large-scale numerical simulation of natural disasters such as an earthquake, tsunami and heavy rain, for Kobe City and other urban areas in Hyogo Prefecture. Besides for the construction of a sophisticated urban area model and the development of new numerical codes, the unit seeks to be a bridge between Science and Local Government for the disaster mitigation and reduction.

Our research unit addressed the following research objects in this fiscal year:

2.1 Development of next-generation urban model for Kobe city

An urban model is used as input data of natural disaster simulation. The reliability of simulations depends largely on the quality of the model. We seek to develop a next-generation urban model for Kobe City; the current model is constructed, based on open-source data of a target area. More detailed data about the urban area, which are managed and maintained by local governments, are to be used to construct the model.

2.2 Numerical simulations for stability analysis of liquefaction

Liquefaction is a kind of disastrous ground failure induced by earthquake. Reliable prediction of liquefaction is of great significance especially for regions near a port where the potential of liquefaction occurrence is high. We develop a finite element method for liquefaction and study the stability of perturbations in the form of plane wave and in the form of spherical wave numerically.

3. Research Results and Achievements

3.1 Development of next-generation urban model for Kobe city

Integrated Earthquake Simulation (IES) requires detailed information about an individual building, such as structure type, construction year and material/structure properties, in order to make a seismic response analysis (SRA) model. External configuration of buildings is stored in commercial GIS (Geographic Information System), but other information is not available unless

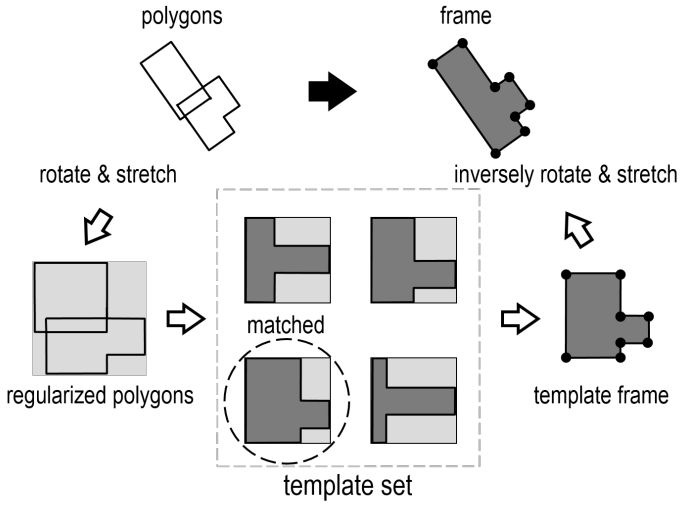


Figure 1. Schematic flow of a template-fitting process.

local government allows us to use their data. With the courtesy of Kobe City Government, we are able to use the data set of some information for registered personal buildings and local government facilities. We are extracting information that is required to make a more sophisticated SRA model from these data sets, and developing a smart program which is capable to handle the data sets to this end. In this fiscal year, we have completed a prototype of such program for the automated construction of an urban area. A new urban area model is made for the city of Kobe, by using this prototype which is applied to multiple data sets of CAD (Computer Aided Design) of structures and building registry of Kobe City.

3.1.1 Template fitting methodology to utilize the CAD data of buildings

In CAD, configuration data of one building are given as a set of polygons. The polygons are independent since it is sufficient for design purpose if they are located at proper positions. No information about connection between polygons is included in CAD. It is a challenging task to utilize CAD data to automatically construct an SRA model, by properly guessing connections of polygons; for instance, a model of finite element method analysis must consist of model elements and those connections.

We have developed a method for automatic construction of a sophisticated SRA model, improving a shape recognition methodology that is based on a template-based floor; see Figure 1. In the developed method, an adequate number of floor arrangements are precomposed as a template set and one of the templates is selected for each floor footprint which is extracted from CAD data; see Figure 2. The advantage of the developed method is that it ensures high robustness in the following two meanings: 1) it can properly convert CAD data to an SRA model;

and 2) it can judge the failure of data conversion due to lack of a proper template.

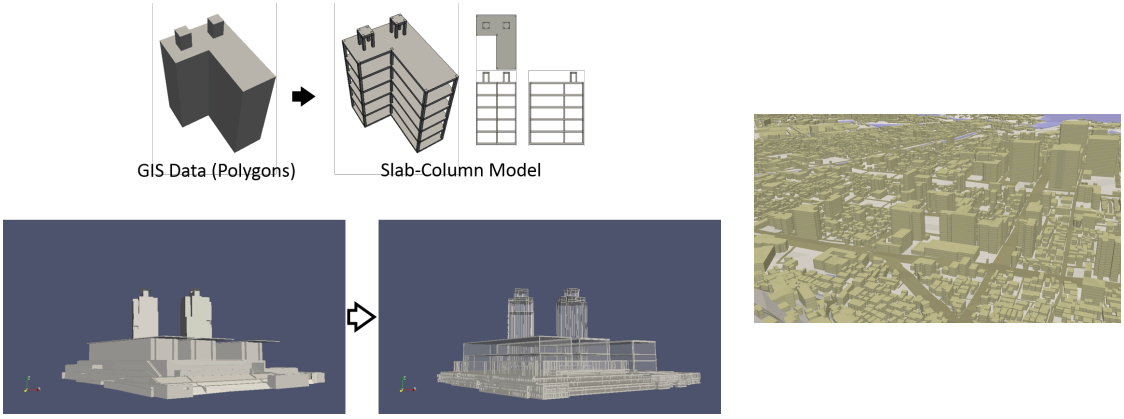


Figure 2. Automatic floor shape recognition against CAD data of buildings.

3.1.2 Utilization of official building registry in urban model

Official building registry provides information about building date, structure type, the number of stories, and so on. Since official building registry is maintained just for taxation in Japan, it often lacks accurate information about the location of individual buildings and cannot be directly utilized for the automatic construction of urban models. We have developed a method to make attribute data of individual buildings with latitudes and longitudes, relating the land identification numbers to the corresponding location on the cadastral map.

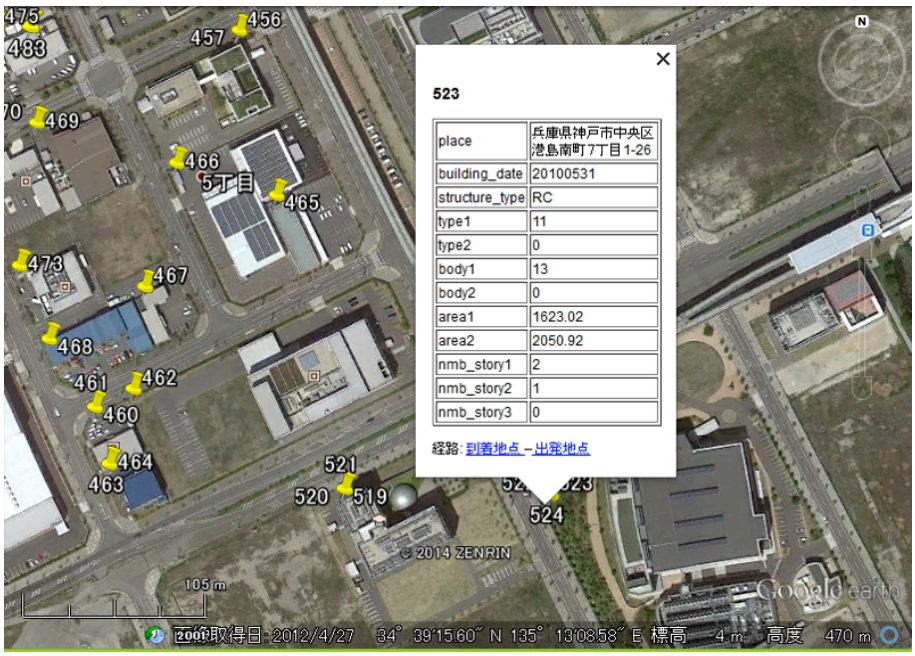


Figure 3. Attribute data of individual buildings with latitudes and longitudes.

Figure 4. Combination results of CAD data and official registry of buildings.

3.1.3 Combination of CAD data and official registry of buildings

Different types of GIS data have different accuracy of location information. Hence, it is not an easy task to accurately combine information stored in different GIS data. We perform proper combining of CAD data with official building registry, in order to construct an urban model of Kobe City; see Figures 3 and 4.

3.2 Numerical simulations for stability analysis of liquefaction

Liquefaction could be regarded as an unstable phenomenon in the sense that shaking induces a sudden transition of ground behavior from solid to liquid. It is a result of non-linear coupling between soil and underground water. We develop a numerical analysis method which is able to capture an unstable solution, to analyze the stability of the governing equations of a coupling problem of soil and underground water.

3.2.1 Mathematical model

As the first step, we study an idealized mathematical model to analyze the stability of a coupling problem solution of soil deformation and water pressure. Denoting by $\boldsymbol{u}$ and p the perturbations of the increments of soil displacement and water pressure, the governing equations of the coupling problem are expressed as

$$\begin{aligned} \rho \mathrm{D}^2 \boldsymbol{u} - \boldsymbol{\nabla} \cdot (\boldsymbol{c} : \boldsymbol{\nabla} \boldsymbol{u}) + \boldsymbol{\nabla} p &= \mathbf{0}, \\ \boldsymbol{\nabla} \cdot \mathrm{D} \boldsymbol{u} - \boldsymbol{\nabla} \cdot (k \boldsymbol{\nabla} p) &= 0, \end{aligned} \tag{1}$$

where ρ, $\boldsymbol{c}$, and k are density, elasto-plasticity and permeability; $\boldsymbol{\nabla}$ and D are spatial and temporal differentiation; and $\cdot$ and $:$ stand for the first and second-order contraction.

Table 1. Material properties for code verification.

	Young's modulus E (MPa)	Poisson's ratio v	Density $\boldsymbol{\rho}$ (kg/m^3)	Permeability $\boldsymbol{k}$ (m^{3}s/kg)
Case 1	50	0.4	2000	1.02e-8
Case 2	32	0.4	2000	1.28e-8
Case 3	12.5	0.4	2000	2.04e-8

3.2.2 Numerical analysis

In the fiscal year of 2012, via theoretical analysis, we show that perturbations in the form of plane wave are always stable if dilatancy is ignored, while, as the degree of dilatancy increases, perturbations in the form of plane wave could propagate in an unstable manner. In this fiscal year, a finite element code for the coupling problem has been fully developed. A key feature of this code is that it is able to model the detaching effect of soil particles, which results in sharp drops in the stiffness of elasticity observed in liquefaction phenomenon. Table 1 summarizes the material parameters which are used in the present numerical analysis.

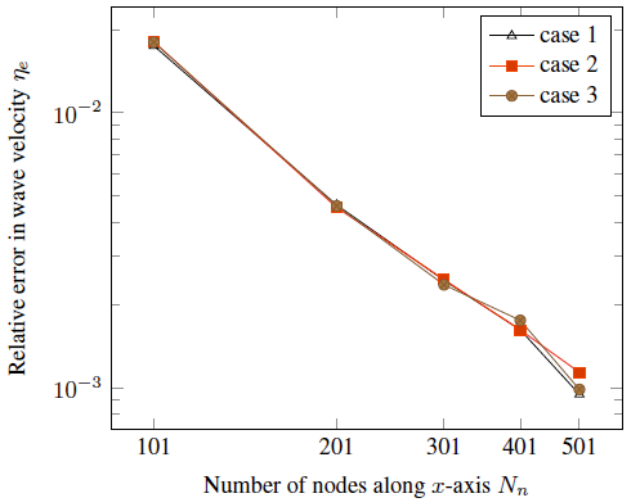


Figure 5. Convergence of wave velocity.

(1) Code verification: Convergence of wave velocity

A closed form expression of the wave velocity is derived for plane wave without dilatancy. We design three test cases of different wave velocities to verify our code. The wave velocities that are computed by using the developed code are in good agreement with the closed form solutions; the relative error in computing the wave velocity converges o as the degree-of-freedom of the model increase; see Figure 5.

(2) Effect of dilatancy in plane wave case

An initial perturbation in the displacement field is prescribed symmetrically at the center of a cubic domain. When the degree of dilatancy is small, the initial perturbation propagates stably from the center to the boundaries of the domain. As the degree increases, unstable solutions are found for the displacement increment and the pressure increment; see Figure 6. The numerical code succeeds to capture this unstable solution of the coupling problem, which we think corresponds to the occurrence of liquefaction.

(3) Spherically symmetric perturbations

For spherically symmetric perturbations, it is difficult to obtain analytical solution for the stability problem. This problem is tackled by the numerical code we developed. For simplicity and to preserve symmetry, initially a perturbation of water pressure is prescribed. When the dilatancy is small, the amplitude of the perturbation decays as it propagates. The solutions of displacement and water pressure are stable. When the dilatancy is large, the perturbation grows exponentially. Unstable solutions of displacement and water pressure are captured; see Figure 7.

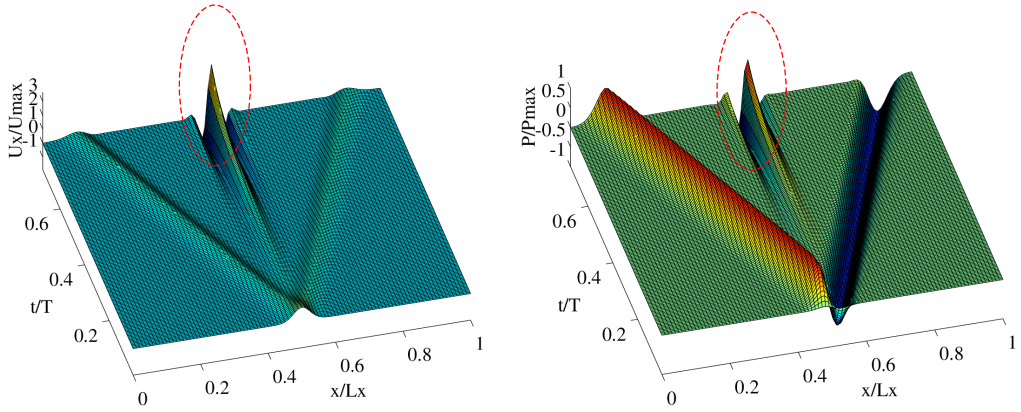


Figure 6. Large dilatancy. Perturbations in the form of plane wave propagate unstably; left) evolution of displacement increment; right) evolution of displacement increment.

(4) Detaching effect:

With the developed numerical code, the detaching of soil particle during liquefaction can be analyzed. Unstable solutions of displacement are suppressed by implementation of detaching. The influence of detaching on pressure changes, whether a detaching criterion is for tensile or compressional stress. As for compression stress, the *loss* in compression stress due to detaching is compensated by an increase of water pressure with respect to the normal (non-detaching) case. As for tensile stress, the stress loss is due to the weakening of tensile stress, which is compensated by the decrease of water pressure. Figure 8 shows the results of the both cases.

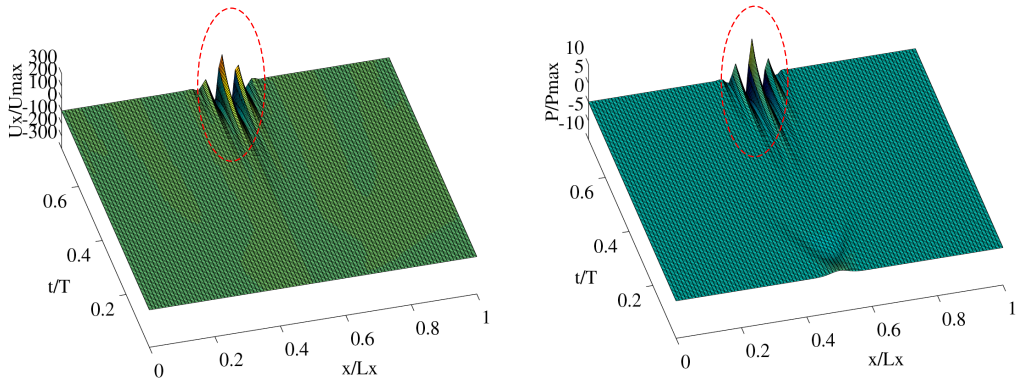


Figure 7. Large dilatancy. Perturbations in the form of spherical wave propagate unstably: left) evolution of displacement increment; right) evolution of displacement increment.

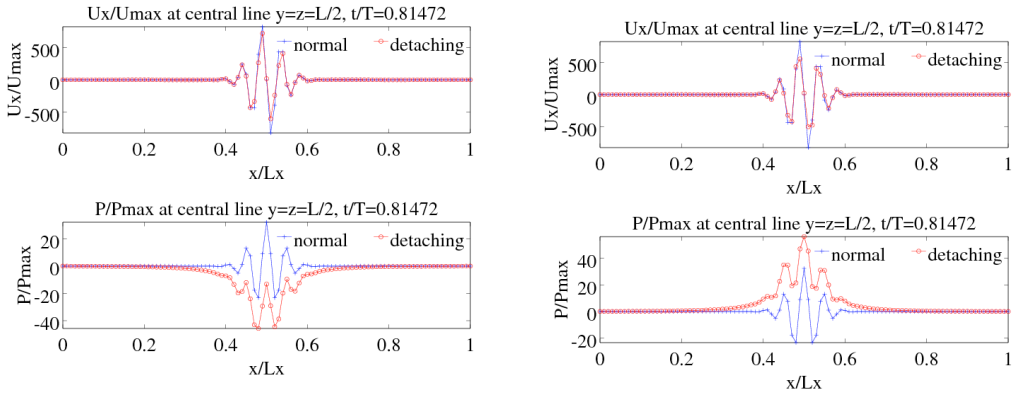


Figure 8. Trial of detaching simulation, solutions along the central line parallel to the x-axis: left) Detaching with respect to tensile criterion; right) Detaching with respect to compression criterion.

4. Schedule and Future Plan

Improvement of the next-generation urban models for Kobe:

In the fiscal year of 2014, we are going to improve the prototype of the next-generation urban model for Kobe City, developing more accurate combination method between different GIS data.

Liquefaction hazards assessment:

In the fiscal year of 2014, we are going to incorporate into IES an advanced finite element code for soil dynamics simulation. Methods to generate ground models and input files from borehole data will be established. Trail run for a target site of Kobe City will be conducted to assess liquefaction hazards.

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] Hideyuki O-TANI, Jian CHEN and Muneo HORI (2013): Smart Visualization of Urban Earthquake Simulation, *Journal of Japan Society of Civil Engineers, Ser. A1 (Structural Engineering & Earthquake Engineering (SE/EE))*, Vol. 69, No. 4.

[2] Hideyuki O-TANI, Jian CHEN and Muneo HORI (2014): A template-based floor recognition applied to 3D building shapes of GIS data, *Journal of Japan Society of Civil Engineers, Ser. A1 (Structural Engineering & Earthquake Engineering (SE/EE))*, Vol. 70, No. 4, accepted.

(2) Conference Papers

[3] Cheng Weishen, Jian CHEN, Hans-Georg Matuttis (2013), Granular Acoustics of Polyhedral Particles, *AIP Conf. Proc.* Vol. 1542, 567-570.

(3) Posters and Presentations

[4] Jian CHEN, Hideyuki O-TANI and Muneo HORI (2013): Stability analysis of liquefaction for plane wave propagation, 68th JSCE Annual Conference.

[5] Jian CHEN, Hideyuki O-TANI and Muneo HORI (2013): Stability analysis of plane wave propagation for investigation of liquefaction triggering condition, The 4th AICS International Symposium.

[6] Hideyuki O-TANI, Jian Chen and Muneo HORI (2013): Template-based automatic construction of building models from GIS data, The 4th AICS International Symposium.

[7] Hideyuki O-TANI, Jian CHEN and Muneo HORI (2013): A template-based construction of seismic response analysis model from GIS data, 33nd JSCE Earthquake Engineering Symposium.

[8] Cheng Weishen, Jian CHEN, Hans-Georg Matuttis (2013), Granular Acoustics of Polyhedral

Particles, Powders and Grains 2013 (The 7th International Conference on Micromechanics of Granular Media).

Computational Structural Biology Research Unit

1. Unit members

Florence Tama (Unit Leader)

Atsushi Tokuhisa (Research Scientist)

Sachiko Kikumoto (Assistant)

2. Research Activities

Biological molecular complexes of such as proteins and RNAs are of great interest in the area of molecular biology as they are involved in cell replication, gene transcription, protein synthesis, regulation of cellular transport and other core biological functions. Those systems undergo large conformational transitions to achieve functional processes. Therefore characterization of structures of these macromolecular complexes is crucial to understand their functional mechanisms, and play an important role in the development of new drugs to treat human disease.

Experimentally, X-ray crystallography has been the primary tool to study protein conformations, providing high-resolution structures. Even though it is at low resolution, cryo electron microscopy (EM) has been providing critical information on structure and dynamics of large biological molecules. More recently, large efforts, such as in Riken/Spring 8 have focused on developing intense X-ray free-electron laser (XFEL) light sources, which offer a new possibility to image single biological macromolecules. Since crystallization is not necessary for such a protein structure analysis, it would be possible to investigate the structure of macromolecular complexes and proteins under various physiological conditions or to observe elementary steps of a biochemical function. However, the technology is still at early stage and it cannot yet achieve atomic level resolution such as obtained by X-ray crystallography.

Computationally, methods have been developed to predict structures from low-resolution data such as cryo-EM either using rigid body fitting or flexible deformations of known atomic structures. In addition, even when structures of the molecules are unknown, atomic models can be predicted using homology modeling and ab initio predictions. While, ab initio prediction still remains difficult for large proteins, success in predicting small proteins have been observed. Finally, algorithms to analyze protein/proteins interactions also have shown success in predicting proteins complexes.

Our research focuses on the development of computational tools to study biological systems,

more specifically, to help in their 3D structural determination using various experimental techniques and to analyze their potential interactions with small molecules in order to design new drugs.

The ultimate line of our interdisciplinary research is too bring experimental data as obtained from X-ray, cryo-EM and XFEL with development and applications of computational tools through the K computer to acquire knowledge on the structure of a physiologically important protein complexes that are unattainable with existing experimental techniques, and to contribute to development of drug design and medical treatment in collaboration with pharmaceutical companies.

3. Research Results and Achievements

3.1. Dynamical information embedded into cryo-EM 2D raw data

Cryo-EM Single-Particle Analysis (SPA) is a method to study the structure and dynamics of macromolecular assemblies. Three-dimensional (3D) structures are computed from a large number of two-dimensional (2D) images collected by transmission electron microscopy. SPA has shown to be promising in capturing heterogeneous conformations of the same macromolecular complex. To study dynamics, a logical solution is thus to acquire EM images of a heterogeneous population of conformations of the same macromolecular complex and then, to use image analysis methods to separate the mixed particles into classes (2 or 3) with similar conformations of particles and, finally, to analyze the 3D structures computed from each of the image classes. This approach is suited if the system is expected to have a few distinct conformations (for example, with and without ligand). However, if the conformational transition is continuous, such approaches cannot capture the intermediate conformations. We developed a new hybrid approach that utilizes molecular mechanics algorithms to simulate conformational dynamics and use the resulting conformations to extract the dynamical information from cryo-EM images. More specifically, a conformational ensemble is generated by molecular mechanics approaches such as normal mode analysis. For each EM image, a conformation that matches most closely is

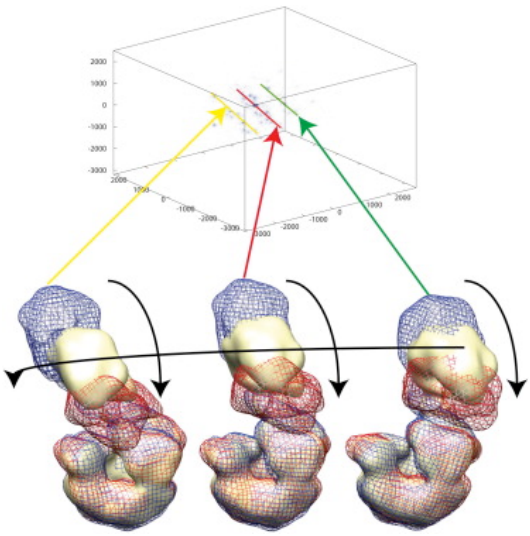


Figure 1. Computed deformation amplitudes projected on to the three most important principal with reconstructed volumetric form of the pseudoatomic structure displaced along the lines yellow, red and green line.

identified (see Figure 1). Through clustering of image/conformation pairs, the 3D conformational variations embedded in EM images are revealed. The performance of the method was shown using synthetic data of two different molecular complexes (*E. coli* 70S ribosome and Tomato Bushy Stunt Virus (TBSV)) and using experimental cryo-EM data of the TBSV.

3.2. Annotating cryo-EM low resolution structure with high-resolution X-ray data

Cryo-EM experiments produces low-to-medium resolution structures (usually in the range between 20 and 4 Å) but allows studying large (diameter larger than 10 nm and molecular weight sometimes of several mega-Daltons) and flexible macromolecular complexes inaccessible to X-ray and NMR techniques. Because the data is at low-resolution, in order to obtain higher-resolution information, know X-Ray structure are often combined with cryo-EM data which is some cases requires X-ray structure deformation (flexible fitting). Flexible fitting of X-ray structure into cryo-EM maps requires first a rigid body fitting of the X-ray structure followed by deformation to fit the density map. In collaboration with Dr. Sugita's team, we have been implementing the algorithms in GENESIS to perform flexible fitting of atomic structures using either full atom or coarse grained model description of the molecule into such low-resolution data. Using generalized ensemble algorithms embedded in GENESIS, such as replica exchange (REMD), the accuracy and efficiency of fittings can be enhanced.

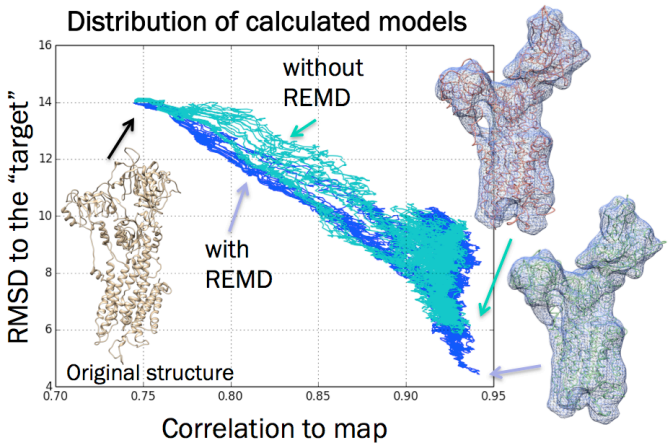


Figure 2. A result of flexible fitting using GENESIS. The original structure is deformed using molecular dynamics simulation to fit the low-resolution data. Fitting with REMD provides structure with better agreement (lower RMSD) with the target structure.

3.3. Computational tools to analyze XFEL experimental data

Since XFEL measurement can be at a single molecular level, and not averaged, its data contains the information regarding the dynamics and conformational variations. In this regard, it is similar to cryo-EM single particle analysis, yet XFEL has a potential to provide more detailed information; it has higher transmissibility and no aberration issue and high resolution is attainable with "diffraction before destruction" effect. We started to explore new methodologies and develop computational tools to analyze XFEL data to extract dynamical

information. This work is in collaboration with Dr. Jonic, CNRS, who has been developing algorithms to analyze 2D images from cryo-EM experiments. The goal is to examine how well XFEL experiments can reveal conformational variations in samples. Simulated diffraction data were generated for incident beams with random orientation for several biological systems adopting several conformations (elongation factor, ribosome, cowpea chlorotic mosaic virus). Similarities in conformation were analyzed for both 2D real image data recovered from diffraction pattern and from diffraction pattern directly. We found that XFEL can differentiate conformation with a 2 Å resolution but that the laser intensity affects the accuracy of detections.

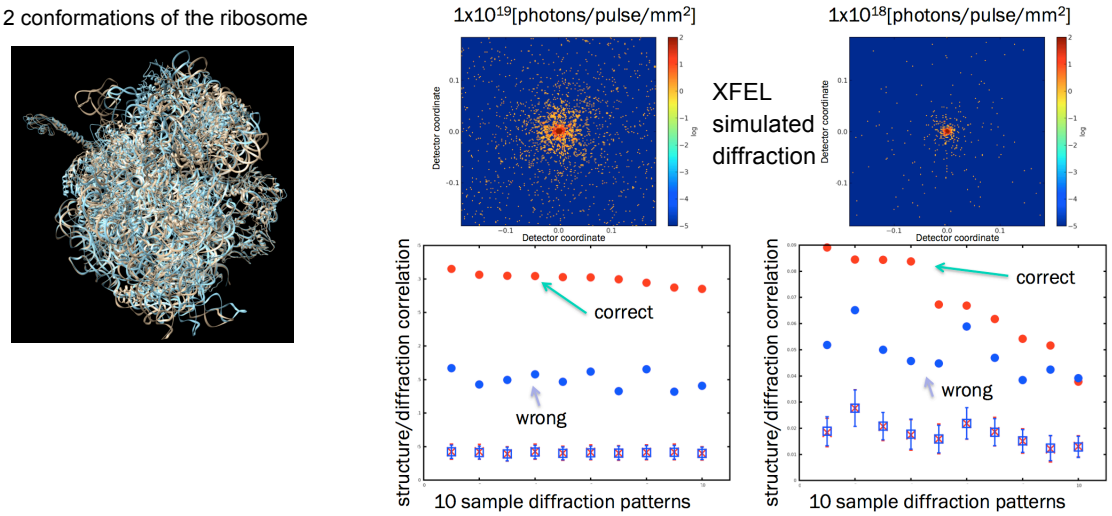


Figure 3. For each 10 sample, the correct conformation shows a higher score (red point) than the wrong conformation/orientation.

3.4. Structure function of proteins, study of small heat shock proteins

The small heat shock proteins (sHSPs) are a virtually ubiquitous and diverse group of molecular chaperones that can bind and protect unfolding proteins from irreversible aggregation. It has been suggested that intrinsic disorder of the N-terminal arm (NTA) of sHSPs is important for substrate recognition. To investigate conformations of the NTA that could recognize substrates, we performed replica exchange molecular dynamics simulations. Behavior at normal and stress temperatures of the dimeric building blocks of dodecamerics HSPs from wheat (Ta16.9) and pea (Ps18.1) were compared because they display high sequence similarity, but Ps18.1 is more efficient in binding specific substrates. In our simulations, the NTAs of the dimer are highly flexible and dynamic, however, rather than exhibiting highly extended conformations they retain considerable α-helical character and contacts with the conserved α-crystallin domain (ACD). Network analysis and clustering methods defined two major NTA conformational forms, designated either "open" or "closed" based on the relative position of the two NTAs in a dimer (see Figure 4).

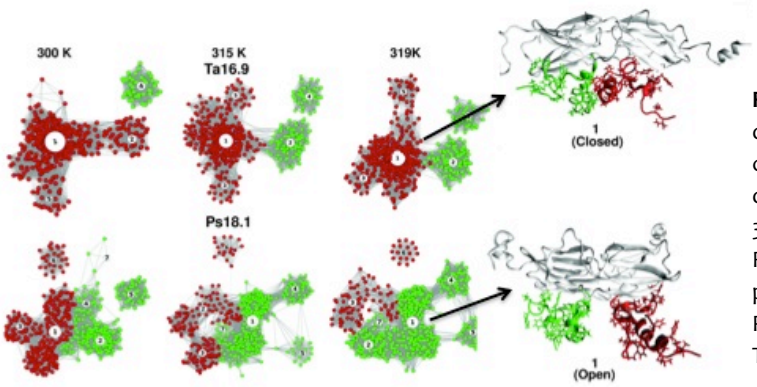


Figure 4. Network representation of open (green) and closed (red) clusters defined by conformations of Ta16.9 and Ps18.1 dimers at 300, 315 and 319 K. Representative structure of the prevalent open conformation of Ps18.1 and close conformation of Ta16.9 are also shown.

The equilibrium constant for a closed to open transition displays significant difference between Ta16.9 and Ps18.1 with the latter one showing more open forms at elevated temperature. The Ps18.1 NTAs are predominantly open and have more hydrophobic solvent accessible surface than the Ta16.9 NTAs, correlated with more effective chaperone activity. NTA hydrophobic patches are comparable in size to the area buried in many protein-protein interactions, which would enable sHSPs to bind early unfolding intermediates. Reduced dimeric interactions of the Ps18.1 NTAs and with the ACD contribute to the differences in dynamics and hydrophobic surface area between the two sHSPs. These data support a major role for the conformational equilibrium of the NTA in substrate binding and indicate features of the NTA that contribute to sHSP chaperone efficiency.

4. Schedule and Future Plan

We plan to continue to develop tools to analyze XFEL data in order to get structural information of biological molecules. In particular, we aim to develop computational algorithms that would provide the shape of the biological molecules. Such algorithms will require the use of simplified representation of the biological molecules as well as a multi-step optimization procedure to build a shape that would be in agreement with the diffraction pattern obtained from XFEL experiments.

In addition, we aim to characterize dynamical information embedded within raw low-resolution data obtained from cryo-EM. This research is an on-going collaboration with Dr. Slavica Jonic (CNRS, Paris). Macromolecular structure determination by cryo-electron microscopy (EM) and single particle analysis are based on the assumption that imaged molecules have identical structure. With the increased size of processed datasets it becomes apparent that many complexes coexist in a mixture of conformational states or contain flexible regions. Algorithms have been developed to yield estimates of voxel-by-voxel variance of a structure reconstructed from the set of its projections. Such variances will be compared from enhanced sampling

molecular dynamics simulations of biological molecules. Such type of approach could later on be extended to data from XFEL experiments as well.

As our research focuses on developing computational tools to analyze low-resolution experimental data, we intend to establish collaborations with experimental groups in Japan and abroad in order to study structure, function and dynamics of biological molecules.

On the longer term we plan to establish methodology to build structure from low-resolution structural data without a priori knowledge of the overall structure of the molecular complexes, since potential targets of the structural analysis by low resolution experimental techniques are multiprotein/RNA complexes. Although it is difficult to acquire the crystal structure of the whole complex, the atomic structure of each component protein and RNA may be known. Moreover, for small proteins, even when there is no structure, their structures can be predicted in relatively high precision using homology modeling. Therefore, if such structures are correctly combined into a model of the complex that fits the three-dimensional electron density map obtained from low-resolution experimental techniques, the atomic structure of a complex could be obtained. A computational framework using multiscale simulations, which would combine the representations at different resolution from all the atoms to coarse-grained representations as well as protein-protein docking algorithms will be developed for such purpose.

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] R. Nogales-Cadenas, S. Jonic, F. Tama, A. Arteni, D. Tabas-Madrid, M. Vazquez, A. Pascual-Montano, CO. Sorzano, "3DEM Loupe analysis of macromolecular dynamics using structures from electron microscopy", Nucl. Acid. Res., (2013) *41:W363-7*.

[2] D. Lyumkis, H. Talley, A. Stewart, S. Shah, CK. Park, F. Tama, CS Potter, B. Carragher, NC. Horton, "Allosteric Regulation of DNA Cleavage and Sequence-Specificity through Run-On Oligomerization", Structure, (2013) *21:1848-58*.

[3] Ahlstrom LS, Baker JL, Ehrlich K, Campbell ZT, Patel S, Vorontsov II, Tama F, Miyashita O., "Network visualization of conformational sampling during molecular dynamics simulation", J Mol Graph Model, (2013) *46: 140-149*.

[4] Q. Jin, COS. Sorzano, JM. de la Rosa-Trevín, JR Bilbao-Castro, R. Núñez-Ramírez, O. Llorca, F. Tama and Slavica Jonić, "Iterative elastic 3D-to-2D alignment method using normal modes for studying structural dynamics of large macromolecular complexes", Structure**,** (2014) *22:496–506*.

(2) Invited Talks

[5] Tama F, "Development of computational tools to characterize structure of biological molecules from low-resolution data", RIKEN joint symposium with INSA, Lyon, France May16th 2013.

[6] Tama F, "Structural modeling from low-resolution experimental data", Workshop on "modeling of biomolecular systems in cellular environments" Kyoto University Oct 31st - Nov 1st, 2013.

[7] Tama F, "Structural modeling of biological molecules from low-resolution experimental data", AICS international symposium, Kobe Dec 2nd-3rd 2013.

[8] Miyashita O, Tokuhisa A, Tama F, "An Overview of Single Biomolecular Imaging by X-ray Free Electron Laser", Institut de Minéralogie et de Physique des Milieux Condensés, France. Dec. 2013.

(3) Posters and Presentations

[9] Q. Jin, C. O. S. Sorzano, J.M. Delarosa-Trevin, J.R. Bilbao-Castro, R. Núñez-Ramírez, O. Llorca, F. Tama, and S. Jonić, "HEMNMA: Hybrid Electron Microscopy Normal Mode Analysis to fully explore continuous-type conformational changes", Cryo-EM 3D Image Analysis Symposium 2014, Lake Tahoe, USA.

[10] Atsushi Tokuhisa, Osamu Miyashita, Florence Tama, "Methodology of a single bio-molecular structure determination for low-resolution data set obtained by X-ray Free Electron Laser", The 51th Annual Meeting of the Biophysical Society of Japan, Kyoto, October 28–30, 2013.

System Operations and Development Team

1. Team members

Fumiyoshi Shoji (Team Head)
Atsuya Uno (Research & Development Scientist)
Hitoshi Murai (Research & Development Scientist)
Motoyoshi Kurokawa (Research & Development Scientist)
Keiji Yamamoto (Postdoctoral Researcher)
Toshiyuki Tsukamoto (Research & Development Scientist)
Fumio Inoue (Research & Development Scientist)
Mitsuo Iwamoto (Technical Staff)
Katsufumi Sugeta (Technical Staff)

2. Research Activities

The K computer is a distributed-memory parallel computer system consisting of 82,944 compute nodes and has played a central role of the High Performance Computing Infrastructure (HPCI) initiative granted by the Ministry of Education, Culture, Sports, Science and Technology (MEXT). HPCI has achieved an integrated operation of the K computer and other supercomputer centers in Japan and has enabled seamless accesses of a cluster of supercomputers including the K computer from users' machines. HPCI has also provided large-scale storage systems which can be accessed from all over Japan.

System Operations and Development Team (SODT) has conducted the research and development on advanced management and operations of the K computer. While analyzing the operational statistics collected during the shared use, SODT has improved the system configuration, such as the job scheduling, the file system, and users' environments. For example, it is very difficult to achieve higher system utilization because the K computer has to process various sizes and types of jobs simultaneously. SODT has responded flexibly to the user's requests and made analysis of the operational status, and then has realized high level utilization approximately 76% in FY2013. Furthermore, SODT has developed tools that support the use of the K computer.

SODT has conducted research in cooperation with the research team of RIKEN Spring-8 Center and RIKEN AICS for big data processing on the K computer. The K computer is used to analyze the huge data transmitted from RIKEN Harima where SACLA XFEL facility is located.

SODT also helps users handle the K computer and utilize the K computer resources effectively by improving the system software. This support has been conducted together with the Software Development Team.

3. Research Results and Achievements

3.1 Improvements of system software of the K computer

We have fixed and improved many points of the system software through the shared use. Here, we describe the main activities in FY2013.

- **Analyzing Operation Statistics and Job Scheduling**

  We have analyzed logs of jobs executed on the K computer and have performed job scheduling simulation using the simulator which can simulate the job scheduling same as real job scheduler on the K computer. Referring these results, we have tuned some parameters of the scheduler (such as scheduling map, file staging timing and so on).

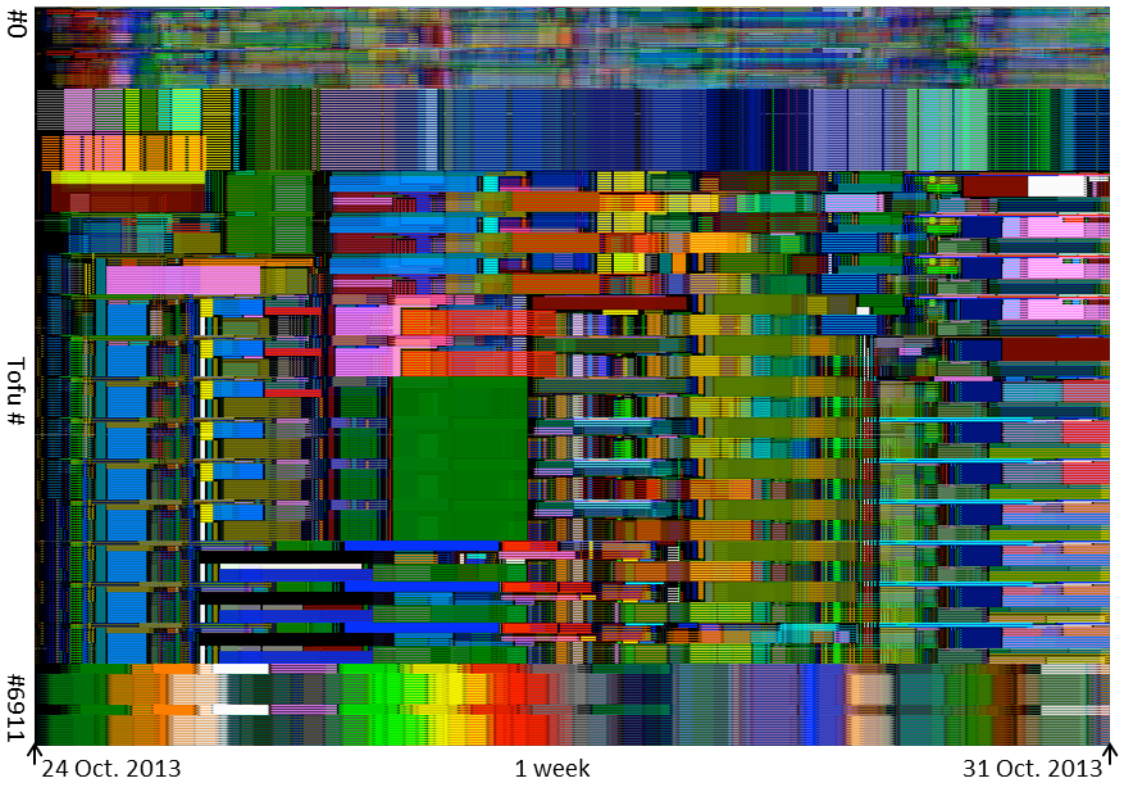


Figure 1. Job execution situation on the K computer.

In order to evaluate the results of the job scheduling, we have visualized the scheduling map. Figure 1 shows the number and size of jobs executed on the K computer during one week from October 24 to October 31, 2013. Since the scheduler allocates a job to nodes shaped a rectangle

in logical 3dimensional coordinate of the K computer, the nodes allocated to one job could be scattered on this figure. The boxes with the same color on the same vertical axis correspond to the same job. The width of a rectangle denotes the elapsed time from the start time to the termination time. The black area shows the nodes either waiting for job execution or for maintenance. The one-ninth of the K computer that corresponds to upper area of this figure is assigned for a resource group "**Small**" which is a limited resource only for small-sized job. On the other side, eight-ninth one is assigned for a resource group "**Large**." As we can see this figure, the K computer can process many jobs in various sizes simultaneously which contributes for high ratio of the node utilization. During this week, approximately 3,600 and 3,000 jobs were processed in **Small** and **Large** respectively, and the total node utilization was approximately 86%.

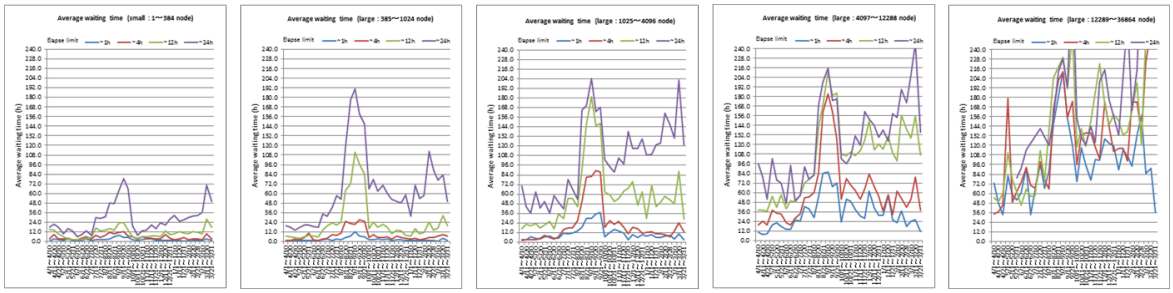


Figure 2. Average waiting time.

Figure 2 shows average waiting times with respect to both job sizes and elapsed times in FY 2013. The average waiting times are directly proportional to both elapsed time and number of nodes. It means that a fairness of opportunity for job execution has been kept.

The average waiting time in September 2013 was very longer than that in other months. Each group had appropriate compute resources for a year, and the resources were divided into two periods: from April to September and from October to March of the next year. In order to consume the remaining compute resources before the resources will be expired many jobs are submitted at the end of the periods. At the job congestion in September 2013 we adjusted system parameters, such as the maximum number of jobs executed simultaneously for each user group and the waiting time has been reduced. But job congestion has occurred for large scale jobs in March 2014. We have to analyze the operational statistics more and need to tune the parameters.

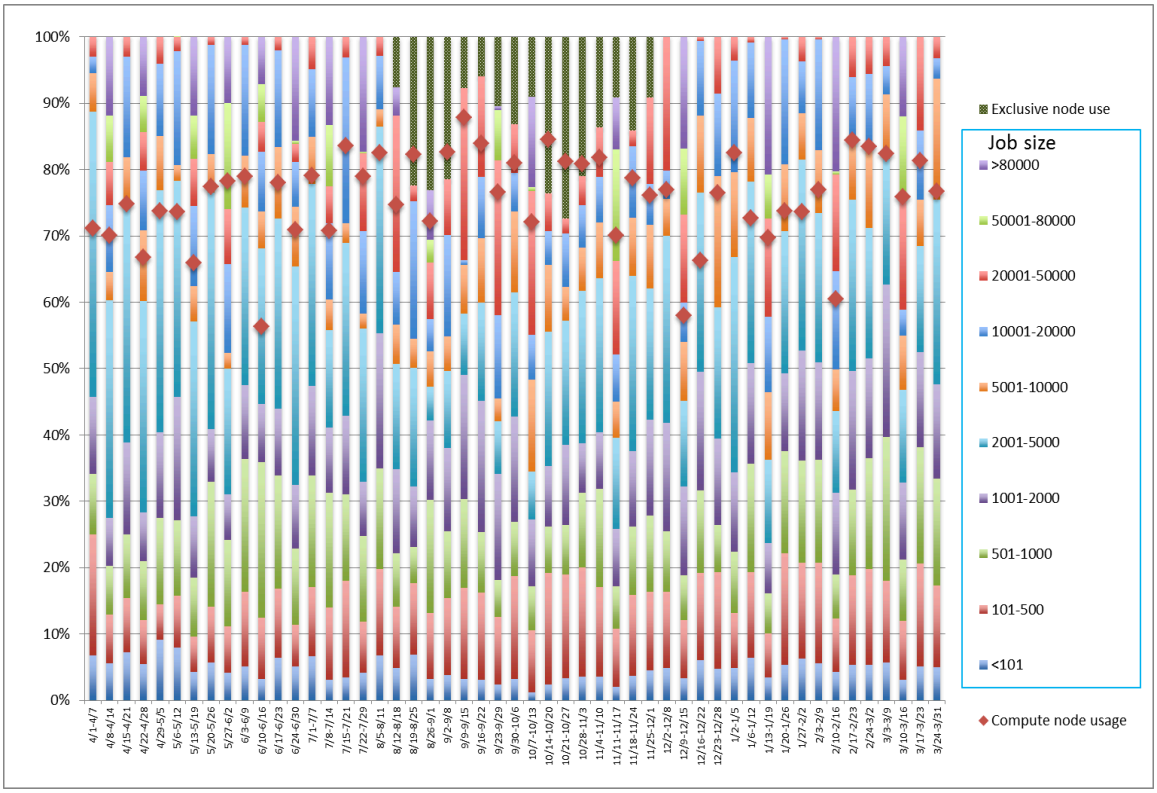


Figure 3. Details of resource usage in FY2013.

Figure 3 shows the compute node usage in FY 2013. We have achieved approximately 76% node usage in FY2013. This is more than 15% higher than last year's.

- **MPI libraries and System tools**

MPI libraries for the K computer are optimized for Tofu interconnect. But most of them are the most effective when 3D torus is specified. Since many jobs on the K computer are executed with 1D or 2D torus we extended some MPI libraries to be able to perform effectively on 1D or 2D torus.

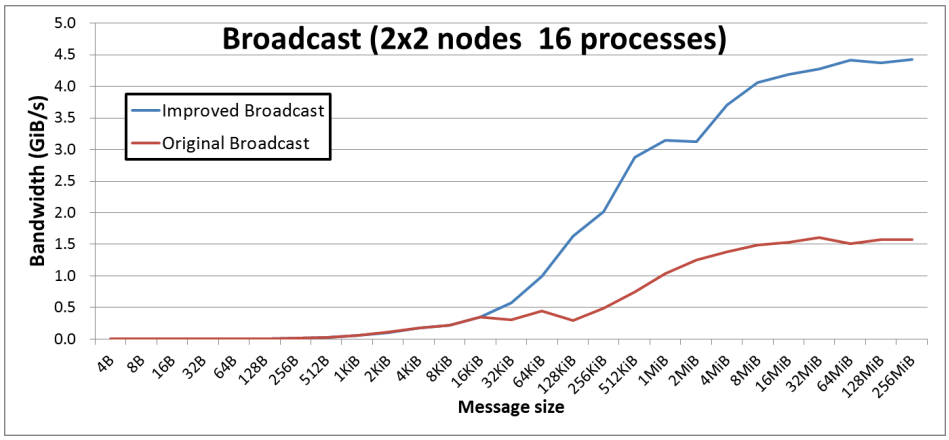


Figure 4. Performance of Broadcast on 2D torus.

Figure 4 shows the performance of original Broadcast and improved Broadcast on 2D torus. This graph indicates that the improved Broadcast is about 5 times as fast as original one using 128KiB message size.

We have developed tools that support the use of the K computer. "Waiting for the K" is a tool that enables users to know the estimated waiting time for the job execution and the available node information of the job execution. We have also been developing another system tools that can enhance the job management. Using these tools, users will be able to submit many jobs at once.

3.2 Cooperative research

- **Big data processing on the K computer**

This research is conducted by collaboration between the RIKEN Spring-8 Center and the RIKEN AICS. The goal of this project is to establish the path to discover the 3D structure of a molecule from a number of XFEL snapshots. Each snapshot size is around 20 Mbytes, but may vary depending on the resolution of image sensor. However, the number of images required to develop a 3D structure of a molecule is millions, resulting 20 PBytes of data size in total. The K computer is used to analyze the huge data. SODT cooperates with the big data transfer from SACLA to the K computer. Further, each image is classified into thousands of images to have every possible snapshot orientations and to reduce the quantum noise.

3.3 User support

We have conducted the user support, such as the user management and the consulting services.

- **User management**

The K computer has 170 or more groups and 2,000 or more users at the end of March, 2014. The number of HPCI users and AICS researchers are approximately 1,750 and 250 respectively. The number of daily active users is approximately 120.

- **Consulting services**

We support users through "the K support desk" and provide users the technical information on the K computer including system environments, system tools, and software libraries. The consulting services have been conducted together with the Software Development Team. Figure 5 indicates the consultation number in FY2013 and the consultation number in FY2013 is approximately 230.

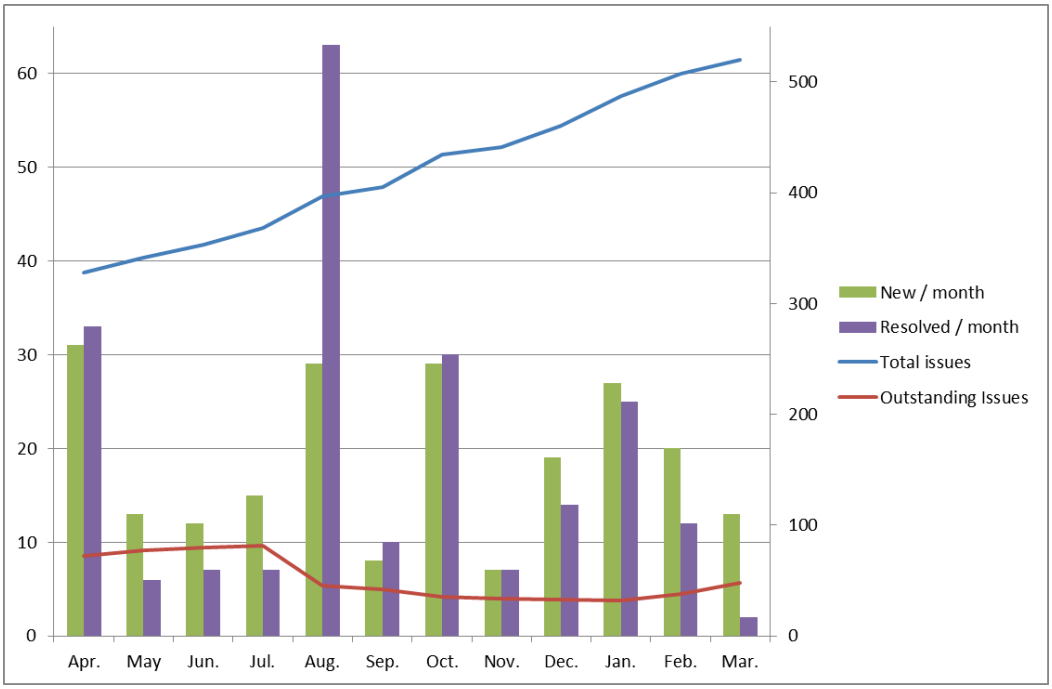


Figure 5. Consultation number in FY2013.

4. Schedule and Future Plan

We continue to improve the system software of the K computer and to provide the user support. The improved system software that supports the use of the K computer will be released in FY2014.

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] Tomoya Adachi, Naoyuki Shida, Kenichi Miura, Shinji Sumimoto, Atsuya Uno, Motoyoshi Kurokawa, Fumiyoshi Shoji, and Mitsuo Yokokawa," The Design of Ultra Scalable MPI Collective Communication on the K Computer", Comput. Sci., 28(2-3):147–155, May 2013.

[2] Fumiyoshi Shoji, "Trend of supercomputer", J.HTSJ, Vol. 52, No220, (2013) 15-20 (In Japanese).

[3] Masaaki Terai, Ken-ichi Ishikawa, Yoshinori Sugisaki, Kazuo Minami, Fumiyoshi Shoji, Yoshifumi Nakamura, Yoshinobu Kuramashi, Mitsuo Yokokawa,"Performance Tuning of a Lattice QCD Code on a Node of the K computer", Transactions of Information Processing Society of Japan, Vol.6, No.3, 43-57 (Sep. 2013) (In Japanese).

[4] Atsushi Tokuhisa, Junya Arai, Yasumasa Joti, Yoshiyuki Ohno, Toyohisa Kameyama, Keiji Yamamoto, Masayuki Hatanaka, Balazs Gerofi, Akio Shimada, Motoyoshi Kurokawa, Fumiyoshi Shoji, Kensuke Okada, Takashi Sugimoto, Mitsuhiro Yamaga, Ryotaro Tanaka, Mitsuo Yokokawa, Atsushi Hori, Yutaka Ishikawa, Takaki Hatsui, Nobuhiro Go, "High-speed

classification of coherent X-ray diffraction patterns on the K computer for high-resolution single biomolecule imaging", In Journal of Synchrotron Radiation, volume 20, 2013.

[5] SHIMIZU Toshiyuki, AJIMA Yuichiro, YOSHIDA Toshio, ASATO Akira, SHIDA Naoyuki, MIURA Kenichi, SUMIMOTO Shinji, NAGAYA Tadao, MIYOSHI Ikuo, AOKI Masaki, HARAGUCHI Masatoshi, YAMANAKA Eiji, MIYAZAKI Hiroyuki, KUSANO Yoshihiro, SHINJO Naoki, OINAGA Yuji, UNO Atsuya, KUROKAWA Motoyoshi, TSUKAMOTO Toshiyuki, MURAI Hitoshi, SHOJI Fumiyoshi, INOUE Shunsuke, KURODA Akiyoshi, TERAI Masaaki, HASEGAWA Yukihiro, MINAMI Kazuo, YOKOKAWA Mitsuo, "Design and Evaluation of K Computer", IEICE TRANSACTIONS on Information and Systems:D, Vol.J96-D No.10 pp.2118-2129,Oct. 2013 (In Japanese)

(2) Conference Papers

[6] Keiji Yamamoto, Atsuya Uno, Hitoshi Murai, Toshiyuki Tsukamoto, Fumiyoshi Shoji, Shuji, Matsui, Ryuichi Sekizawa, Fumichika Sueyasu, Hiroshi Uchiyama, Mitsuo Okamoto, Nobuo Ohgushi, Katsutoshi Takashina, Daisuke Wakabayashi, Yuki Taguchi, Mitsuo Yokokawa, "The *K computer Operations: Experiences and Statistics", International Conference on* Computational Science (ICCS), 2014, Australia. (to appear)

(3) Invited Talks

[7] Fumiyoshi.Shoji, “Introduction to the K computer”, The K day in MQM 2013.

Software Development Team

1. Team members

Kazuo MINAMI (Team Head)
Masaaki TERAI (Research & Development Scientist)
Atsuya UNO (Research & Development Scientist)
Akiyoshi KURODA (Research & Development Scientist)
Hitoshi MURAI (Research & Development Scientist)
Kiyoshi KUMAHATA (Research & Development Scientist)
Shunsuke INOUE (Research & Development Scientist)
Yukihiro HASEGAWA (Research & Development Scientist)

2. Research Activities

The K computer is one of the most massively parallel supercomputers in the world. In order to utilize and operate the K computer efficiently, it is important to develop performance improvement techniques and to enhance middleware capabilities well suited to K computer's large-scale concurrency. We developed some techniques for performance improvement by examining several actual applications in various science fields. We also evaluated the K computer middleware and obtained several issues to be improved.

We have performed the following activities this fiscal year.

i. Verification of computational capabilities of the K computer by measuring performance of some kernel codes extracted from real applications such as FrontFlow/blue, NICAM, and PHASE
ii. Technical support to the Registered Institution for Facilities Use Promotion or RIST and to users who conduct research on enhancement of the K computer capabilities
iii. Evaluation of middleware of the K computer to clarify weak points to be refined in the next release of the middleware.
iv. Development of original middleware such as K-scope, KITRA, and a visualization tool of TofuPA.

We have also studied performance tuning of high performance conjugate gradient method (HPCG) that is a candidate for ranking high performance system as a substitute for LINPACK benchmark program.

The details of our activities are described in the following sections.

3. Research Results and Achievements

3.1. Performance Tuning of Applications

3.1.1 Identification of performance degradation of FrontFlow/blue and NICAM

We found two kinds of performance degradation in execution of an application FrontFlow/blue that had not been reported before and tracked down these issues. One was that it took much longer time for a specific input data than for any other data. The other one was that multiple measurement time for the same input data was not constant but fluctuated, though it was expected to be constant. After careful and precise investigation, we found that. dynamic memory allocation and de-allocation were carried out frequently for the specific input data in the former case, and the application program should be modified not to issue frequent memory operations. As for the latter case, a daemon called "pdflush," which writes calculated data onto hard disks and is executed at an appropriate period, took time in one of the multiple processes and this cannot be controlled by application users because the daemon was controlled by operating system. The timing of invoking the pdflush should be synchronized for every process by any means.

The Non-hydrostatic Icosahedral Atmospheric Model (NICAM) is an application for simulating global climate. It consists of two parts; one is calculation of global convection on the basis of fluid dynamics and the other one is calculation of phase transitions based on cloud microphysics. We found that the numbers of floating-point operations in parallel tasks varied widely, then load imbalance among the parallel tasks was occurred. We are studying how to suppress load balance for the code.

3.1.2 Efficient use of the six-dimensional Tofu interconnect

Communication costs in applications become relatively higher with the increasing the number of parallel processors, and therefore parallel efficiency becomes worth for large scale jobs. We found an efficient use of the six-dimensional Tofu interconnect, which provides multiple routes among compute nodes.

To obtain higher performance on the K computer, hybrid parallelization with threads and MPI parallelization and two-way parallelization were found to be efficient for some applications. Two-way parallelization means that application is parallelized in two disjoint discretization spaces, e.g. wave functions and energy bands in the density functional theory application PHASE. Thanks to the Tofu interconnect, we succeeded in mapping these two parallel directions onto two orthogonal MPI communicators, respectively, each of which is three-dimensional mesh network topology, by the following;

1. appropriate MPI rank mapping by the specified mapfile,
2. dynamic allocation of sub-communicators by using a six-dimensional rank query tool which is specific for the K computer.

We found that communication time in three-dimensional FFT and diagonalization of PHASE halved and obtained good total performance.

3.1.3 Development of a benchmark suite for checking degradation of compilers

It is important to check whether system performance is improved or not after updates of system software, such as OS kernel, compilers, and libraries, are carried out with the improved and/or bug-fixed version. It sometimes induces performance degradation without any noticing.

We developed a tool to check whether computation performance of applications degrade or not by comparing computation time of a suite of applications on a new system environment with that on the previous one. It can detect the degradation by measuring computation time of several applications. By checking the performance, we can decide whether the updated system environment should be open to users or not.

We found the compiler version K-1.2.0-15 gave performance degradation to two applications, NICAM and PHASE, by using the check suite tool and we could pull the release of the version off. We are extending the tool to check other system software.

3.1.4 Evaluation of a mechanism for automatic measurements of performance

In order to operate the K computer efficiently, it is important to analyze properties of jobs that are submitted and run on the K computer. We tested a method to collect application characteristics automatically and evaluated the feasibility to collect hardware counter information and performance information during system operations. We also evaluated negative impacts of the data collection because such a data collection may affect system operations and application performance. According to our analysis, automatically collected results for execution time, memory throughput, and performance of floating-point operations were consistent with manually collected results from precision performance analyzer function data. Thus, we conclude that our collecting method provides results with sufficient accuracy and without negative impact for the system operations. However, when file I/O occurred during measurement the results tend to deviate from the correct value. We plan to evaluate the flat MPI model using multiple processes within a node, so we need to establish an evaluation method for those situations.

3.1.5 Evaluation of flat MPI applications

We observed that electric power consumption exceeded the limit while a flat MPI application was executed on the full system of the K computer. The total amount of memory access of the flat MPI application was found to vary largely according to the number of MPI processes in an LSI socket, on which there rare eight cores. We concluded that memory access by the flat MPI application on the full node produced large power consumption. Though we have to analyze the relation between power consumption and executions of flat MPI applications more precisely, such the applications should be treated more carefully when they are run on the full node for the meanwhile.

3.2 User Support

We provide a user support service named "K support desk" for the Registered Institution for Facilities Use Promotion, or Research Organization for Information Science and Technology (RIST) and for users who conduct research on enhancement of the K computer capabilities. The total number of inquiries was approximately 1500. The system was improved according to some requests.

We regularly held meetings with RIST as part of the service, in which we discussed application porting to the K computer, numerical methods, and performance analysis. We could share skills and experiences each other through the meetings, and exchanged and resolved technical issues related to improving application performance.

3.3 Classification of Applications and Evaluation of the K computer Middleware

We classified optimization methodology by examining typical kernels appeared in user applications. We also evaluated and developed middleware programs such as compilers, mathematical libraries, and programming support tools. The details are described below.

3.3.1 Run-time characteristics of user applications

Keys for improving user applications efficiently are to uncover the potential parallelizability in application programs and make use of features of processor core as much as possible.

Firstly, we classified user procedures such as functions, subroutines, and loops into 19 kernels listed in Table1 according to six measures of byte/flop value, data locality, inter-iteration dependency of loops, loop body size, thread parallelizability, and process parallelizability. Selected kernels are listed in Table 1. Then we selected part of applications as representative kernels, each of which consumes a short computation time.

Secondly, we evaluated kernel characteristics in computations by using hardware performance counter information. Finally, we developed a particular method for thoroughly bringing out the potential parallelizability of each kernel and an optimal method to improve the kernels.

Table. 1 Selected kernels from representative application programs

Applications	Kernels	Features
Structural analysis code by FEM	Quadruple precision FMA	Matrix multiplication, no multi-threading
	Heat flux evaluation	Matrix multiplication, no multi-threading
Semiconductor analysis	The function for OpenMP multi-threading	Forking to outside of a parallel region
	Timer routine	Using the clock function in the standard library
	Dot function	Small loop body, small number of loop iterations
	The region generating coefficients matrixes and the region updating physical parameters	Small number of loop iterations, large number of IF statements
	The upper loop region in setLRAV	Using pointers to the other pointer variables
	updateModelSemiConAV	Large loop body, loop includes IF statements
Fluid analysis code OpenFOAM	Avg	Using vector
	Centre	Using templates
	findSharedBasePoint	Using templates
	simpleFoam	Small loop body, no inter-iteration dependency loop
Hartree-Fock method in Quantum chemistry	Two-electron integral kernel	Large loop body, small number of loop iterations
	Dynamic allocation of array variables	All threads concurrently issue malloc instructions for allocating small memory space
Weather and climate simulation code	Evaluation of deposition and melting	Large loop body, no software pipelining, SIMD not effective
	Evaluation of water state transition in atmosphere	Large loop body, no software pipelining, SIMD not effective
	Terminal velocity evaluation	Small loop body, partial software pipelining, SIMD effective
Fluid analysis code by FEM	Subroutine grad3x	Arithmetic only kernel (I/O instructions not included)
	Subroutine gdcomx	Kernel for inter-node communications

3.3.2 Findings of deficiency of compiler capabilities

Compilers should generate optimized codes that make use of CPU features at a maximum. However, present compilers do not always generate the codes so as to bring out those features

due to compilers analysis deficiency. We analyzed codes generated by compilers and studied how to write source codes to obtain faster object codes. Some findings were deficiencies in optimizing loop exchanges, loop blocking, in-line expansion functions, and software pipelining functions. We also found out that an intrinsic function SQRT of Fortran should be used to obtain higher performance, instead of a direct statement of the power of 1/2 in a source program.

We also listed issues to be improved in the next release of middleware and requested the improvement to Fujitsu Ltd.

3.3.3 Development of tools for the K computer

We studied three middleware tools that are efficient to improve user programs on the K computer. Those are a Fortran static analysis tool "K-scope", a cache memory emulation software "KITRA", and a visualization tool of performance information of Tofu.

A) K-scope: Fortran static analysis tool

We have to understand the structure of an application program, when we want to improve performance of the program. We developed a static analysis tool for Fortran source program, called K-scope, by which the structure such as loops, conditional branches, and procedure calls can be displayed as a tree structure. The tools have already been opened via our web site as open-source software under the Apache license version 2.0.

We improved and enhanced the tools this year as follows:

1. Visualization function of performance profiling data
   To identify bottlenecks of application programs, we have to analyze both source code and performance-profiling data. We added a feature for analyzing performance-profiling data that is based on the visualization of Fujitsu profiling data together with the source code.
2. Provision of a remote server for parsing source code (This work was done in collaboration with the HPC Usability Research Team in AICS.)
   K-scope uses an intermediate code generated by the XcalableMP compiler to offload a parsing of the Fortran source code. However, a binary package of XcalableMP is only available for major Linux distributions, and it is quite difficult for application users to install the XcalableMP compiler on their environments. To resolve this problem, we developed an offloading mechanism that uploads the source code, parses it on a remote server on which XcalableMP is installed, and then imports the intermediate code to K-scope.

B) KITRA: Cache memory emulator

We can obtain a rough behavior of an application program executed on the K computer by

several profiling tools. Especially, a precise PA tool, which can measure some hardware behavior such as the number of floating-point operations and total number of cache miss hit in a specified range of the code. However, information of cache miss hit of every array variable cannot be provided. To improve performance of the code, we have to know cache replacement behavior in detail.

We developed a cache memory emulation software "KITRA", which allocates a small memory buffer working as a cache memory. It emulates a least recently used (LRU) algorithm for controlling cache miss/hit. When a load/store operation is executed for some variables in an application, KITRA captures the source/destination memory addresses of the variables, and it emulates the cache miss/hit on its own buffer using the LRU algorithm. The detailed cache miss/hit information is reported with the line number of the source code and the name of the array in which the memory access occurred. We are now evaluating a preliminary version of KITRA by applying it to several kernels of actual applications.

C) Prototype tool for visualization of TofuPA

TofuPA provides us information of hardware counter regarding message traffics on the Tofu interconnect. It includes physical coordinates of a six-dimensional mesh/torus network. We have developed the visualization tool of TofuPA in 2012. It can displayed all of the traffics on the Tofu interconnect, but we need to know traffics of each application which is run on a part of the K computer.

This year we improved the tool so that it can display the traffics of each job as well as MPI rank mapping information. This tool is efficient to improve application performance as high as possible by controlling communication paths and communication order to reduce communication conflict. However, it is quite complicated to use for general users. Therefore, we studied how to apply the tool to applications and gave users a guideline of communication optimization by using the tool.

3.4 Study on a novel benchmark program HPCG for supercomputers

We evaluated and optimized a novel benchmark program HPCG for supercomputers on the K computer. This program can measures performance information of a supercomputer using the preconditioned conjugate gradient (CG) method to solving a system of linear equations, in which the coefficient matrix is sparse. Unlike the famous conventional benchmark program LINPACK, the score from HPCG depends on not only CPU performance but also memory and network bandwidth. We obtained a pre-released version of HPCG code before its official announcement at SC13 and examined it. We achieved speedup of twelve times in terms of total

calculation time by applying several improvement techniques to original code. Our results were reported by the proponent of HPCG at SC13. We have invited to the HPCG special workshop held on March 2014 and presented the results in detail.

4. Schedule and Future Plan

Our activities aim at providing an environment in which users can obtain high capabilities of the K computer easily. To realize this, we will continue to study and evaluate characteristics of the K computer hardware and applications from viewpoints of computer science. We also improve the middleware on the K computer.

5. Publication, Presentation and Deliverables

(1) Journal Papers

[1] Y. Hasegawa, J. Iwata, M. Tsuji, D. Takahashi, A. Oshiyama, K. Minami, T. Boku, H. Inoue, Y. Kitazawa, I. Miyoshi, M. Yokokawa, "Performance evaluation of ultra-largescale first-principles electronic structure calculation code on the K computer", The International Journal of High Performance Computing Applications, published on October 17, 2013 as doi:10.1177/1094342013508163

[2] K. Kumahata, S. Inoue, K, Minami, "Performance Tuning for Gradient Kernel of the FrontFlow/blue on the K computer", IPSJ Transactions on Advanced Computing Systems, Vol.6, No.3, pp.31-42. (September, 2013). (in Japanese)

[3] M. Terai, K. Ishikawa, Y. sugisaki, K. Minami, F. Shoji, Y. Nakamura, Y. Kuramashi, M .Yokokawa, "Performance Tuning of a Lattice QCD Code on a Node of the K computer", IPSJ Transactions on Advanced Computing Systems, Vol.6, No.3, pp.43-57. (September, 2013). (in Japanese)

[4] A. Kuroda, Y. Sugisaki, S. Chiba, K. Kumahata, M. Terai, S. Inoue, K. Minami, "Performance Impact of TLB on the K computer Applications", IPSJ Transactions on Advanced Computing Systems, Vol.6, No.3, pp.1-11. (September, 2013). (in Japanese)

[5] S. Inoue, S. Tsutsumi, T. Maeda, K. Minami, "Performance Optimization of Seismic Wave Simulation Code on the K computer", IPSJ Transactions on Advanced Computing Systems, Vol.6, No.3, pp.22-30. (September, 2013). (in Japanese)

(2) Conference Papers

[6] K. Kumahata, S. Inoue, K. Minami, "Kernel performance improvement for the FEM-based fluid analysis code on the K computer", Procedia Computer Science Vol.18 2013 International Conference on Computational Science, pp.2496-2499. (June, 2013).

[7] M. Terai, K. Ishikawa, Y. Sugisaki, K. Minami, F. Shoji, Y. Nakamura, Y. Kuramashi and M. Yokokawa, "Performance Tuning of a Lattice QCD code on a node of the K computer", High

Performance Computing Symposium 2013, (January, 2013). (in Japanese)

[8] S. Inoue, S. Tsutsumi, T. Maeda and K. Minami, "Performance optimization of seismic wave simulation code on the K computer", High Performance Computing Symposium 2013, (January, 2013). (in Japanese)

[9] K. Kumahata, S.Inoue and K. Minami, "Performance Tuning for Gradient Kernel of the FrontFlow/blue on the K computer", High Performance Computing Symposium 2013, (January, 2013). (in Japanese)

[10] A. Kuroda, Y. Sugisaki, S. Chiba, K. Kumahata, M. Terai, S. Inoue and K. Minami, "Performance Impact of TLB on the K computer Applications", High Performance Computing Symposium 2013, (January, 2013). (in Japanese)

[11] Y. Hasegawa, K. Kondo, et al., "Performance evaluation of the commercial general-purpose finite element analysis application on the K computer", JSCES, Tokyo, (June, 2013). (in Japanese)

[12] A. Kuroda, N. Oi, H. Inoue, H. Murai, T. Yamasaki, T. Ohno, T. Imamura and K. Minami, "Communication Optimization Method on a High-dimensional Mesh / Torus Network for Real Applications – Case Study for the Tofu Network of 'K computer' –", High Performance Computing Symposium 2014, (January, 2014). (in Japanese)

(3) Invited Talks

[13] Y. Hasegawa, "Toward Petaflops Applications - First-principles electronic structure calculation program RSDFT -", HPC Strategic Program Field 5 "The origin of matter and the universe" Symposium, (March, 2013). (in Japanese)

[14] A. Kuroda, "Example of Utilization of the K computer - With Optimization of PHASE", The Society of Polymer Science, Research Group on Computational Polymer Science, (March, 2013). (in Japanese)

[15] M. Terai, "Introduction to Analysis Tool for Fortran Code with XcalableMP Intermediate Code", 1st XcalableMP Workshop, (November, 2013). (in Japanese)

(4) Posters and Presentations

[16] M. Terai, E. Tomiyama, H. Murai, K. Kumahata, S. Hamada, S. Inoue, A. Kuroda, Y. Hasegawa, K. Minami and M. Yokokawa, "Development of supporting tool "K-scope" to tune of Fortran code", High Performance Computing Symposium 2013, (January, 2013). (in Japanese)

[17] S. Inoue, S. Tsutsumi, T. Maeda, K. Minami, "Performance Evaluation and Optimization for Memory-Intensive Application in the K computer", SACSIS 2013, (May, 2013). (in Japanese)

[18] T. Yamasaki, J. Nara, J. Koga, T. Uda, A. Kuroda, K. Minami and T. Ohno, "Planewave Based First-Principles Calculations on the 83000 Nodes K-Computer Applied to SiC Screw Dislocations", 2013 JSAP-MRS Joint Symposia, (September, 2014).

[19] T. Yamasaki, J. Nara, J. Koga, T. Uda, A. Kuroda, K. Minami and T. Ohno, "Geometric and Electronic Structures of Threading-Screw-Dislocations in 4H-SiC", 22nd Meeting on SiC and Related Semiconductors, (December, 2013). (in Japanese)

[20] T. Yamasaki, H. Koyama, J. Nara, J. Koga, T. Uda, A. Kuroda, K. Minami and T. Ohno, "4H-SiC Screw Dislocations and Their Electronic Structures", 2013 International Conference on Solid State Devices and Materials, (September, 2013).

(5) Patents and Deliverables

[21] K-scope: Fortran source code analysis tool–visualization source code structure and performance profiling data –, (April, 2013).

Computer simulations create the future

RIKEN Advanced Institute for Computational Science

ANNUAL REPORT

FY2013-14

7-1-26, Miatojima-minami-machi, Chuo-ku, Kobe, Hyogo 650-0047 Japan

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

RIKEN2014-043