AICS

RIKEN Advanced Institute for Computational Science

ANNUAL REPORT

FY2014

AICS Research Activities

RIKEN
Advanced Institute for
Computational Science

Contents

Part II: Operations and Computer Technologies Division

Part III: Exascale Computing Project

Preface

This report presents the research activity of RIKEN Advanced Institute for Computational Science (AICS) for the period of 1 April 2014 to 31 March 2015.

This is the fifth year for AICS since its foundation in 2010. The Research Division continued to operate with 16 teams and 3 units as established in 2012, and so did the Operations and Computer Technologies Divisions with 4 teams.

A major organizational addition is the Exascale Computing Project Division with 4 teams in April 2014. The post K computer project, now officially named *Flagship2020 Project*, started in JFY2014. RIKEN and AICS is charged with the development of the post K computer, and this division was set up to carry out the development. As of 1 April 2014, the number of researchers in the three Divisions was 130 in total.

The activities of all three Divisions are compiled in this volume. They resulted in 111 journal papers, 95 conference reports, 130 invited talks, 265 posters and presentations, and 41 patents and deliverables.

Memorable awards bestowed upon AICS researchers included No. 1 and No.2 ranking on Graph500 in June and November 2014, respectively, No.1 in HPC Challenge Class2 and No. 2 on HPCG ranking both in November 2014. They continued to illustrate the well-balanced and versatile performance of the K computer in its 3rd year of operation.

Many research-related events took place in this fiscal year. The 5th AICS International Symposium, which became an annual event at Kobe, was held on 8 – 9 December 2014 under the title "Computer and Computational Sciences toward Exascale Computing". AICS also hosted two major conferences; "JST/CREST International Symposium on Post Petascale System Software" on 2 – 4 December 2014, and "4th International Symposium on Data Assimilation" on 23 – 27 February 2015.

The international research scope was expanded through an exchange of MOU with *Maison de la Simulation* at the French Embassy in Tokyo on April 2014, and by joining

the *Joint Laboratory toward Extreme Scale Computing* (JLESC) in spring 2015.

We hope that this volume conveys the excitement of research and development at the forefront of computational and computer science being conducted at RIKEN AICS to readers.

July 2015

Akira Ukawa
Deputy Director
RIKEN Advanced Institute
for Computational Science

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) put 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 constructed the K computer. The K computer is a shared resource based on the above law and, with its wide accessibility, is being 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),
- Mentoring 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).

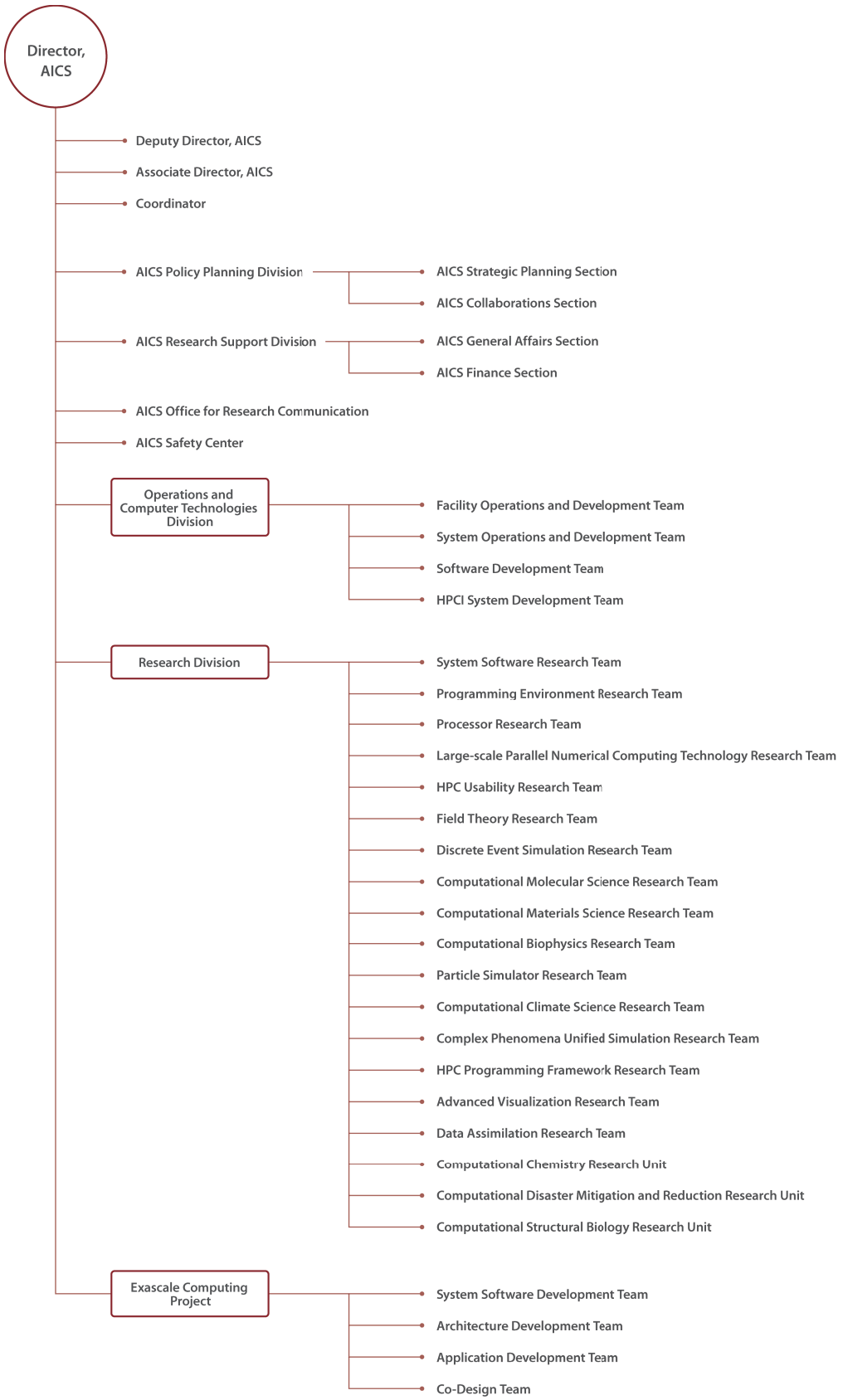
The AICS researchers are carrying out the leading edge research of computational science and technology, and also expected to provide useful software to the users of the K computer.

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.

AICS 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.

Organization



System Software Research Team

1. Team members

Yutaka Ishikawa (Team Leader)
Atsushi Hori (Senior Scientist)
Yuichi Tsujita (Research Scientist)
Keiji Yamamoto (Postdoctoral Researcher)
Kazumi Yoshinaga (Postdoctoral Researcher)
Akio Shimada (Research Associate)
Masayuki Hatanaka (Research Associate)
Norio Yamaguchi (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, and fault-aware operating system for next-generation supercomputers based on many core architectures.

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, weather and climate models developed at RIKEN AICS, includes the multiple stencil computations. 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, which 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. Therefore, our previous work has developed an RDMA-transfer scheduling algorithm, called *Modified-Bottom-Left*, to avoid the congestions on physical network links and the conflicts of receiver-side RDMA engines. In the latest MPI specification version 3.0 (hereafter referred to as "MPI-3.0"), neighborhood collective primitives were introduced. For example, the MPI_Neighbor_alltoallw primitive is a neighborhood collective version of MPI_Alltoallw. These primitives communicate with the user-defined processes instead of all participants on the communicator. Also, non-blocking collective primitives such as MPI_Ineighbor_alltoallw primitive are introduced in MPI-3.0. To support MPI-3.0 on K computer, we are porting MPICH-3.1, which is one of the major MPI implementations. Since the default neighborhood collective implementation in MPICH-3.1 is a generic implementation, we develop the optimized implementation of neighborhood collective on Tofu interconnect using our RDMA-transfer scheduler.

Proposal of RDMA-based collective communication, Cached-Multi-W

If all point-to-point user-data transfers defined in a neighborhood collective communication are replaced by RDMA Write (or RDMA Read) transfers as a whole, the RDMA-based transfers can progress the non-blocking collective communication without CPU intervention, and reduce extra copy overheads and memory consumption for data transfers due to the Zero-Copy feature. Therefore, an RDMA-based approach, called *Cached-Multi-W*, is proposed to further reuse a cached series of RDMA descriptors. In this approach (see Figure 1), once a neighborhood collective communication function such as MPI_Neighbor_alltoallw() is called, the arguments and a series of RDMA (Write) descriptors corresponding to the collective communication pattern are cached as a reusable entry. And then if the subsequent collective calls match the arguments with a cached entry, the calls reuse a cached series of RDMA descriptors, instead of generating and scheduling the RDMA descriptors.

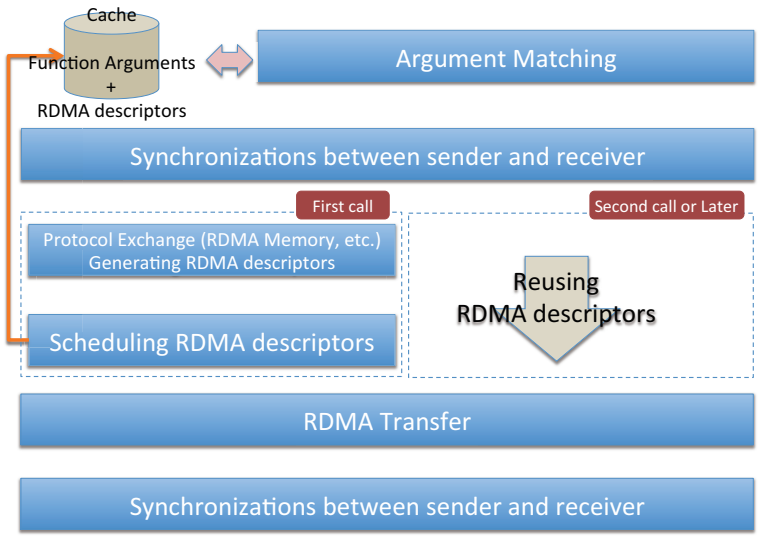


Figure 1 Cached-Multi-W (Cached Multiple RDMA Writes) approach

Implementation and Evaluation

The proposed *Cached-Multi-W* approach has been implemented for MPI_Neighbor_alltoallw() in MPICH-3.1 on K computer. This implementation uses a generator and scheduler of RDMA descriptors developed in PRDMA (Persistent Remote Direct Memory Access).

We measured two MPI_Neighbor_alltoallw implementations in a ghost cell exchange: (1) MPICH default implementation, and (2) the proposed Cached-Multi-W implementation. The communication pattern is a ghost cell exchange for two dimensional 9-point stencil computation, the cell size is 800 bytes (MPI_DOUBLE × 100), the ghost width is 2, and the cell shapes per process are 8x8, 16x16, and 32x32. In Figure 2-1 and Figure 2-2, the horizontal axis shows each call of MPI_Neighbor_alltoall(). The vertical axis shows the elapsed time for a call. The proposed Cached-Multi-W implementation is up to 77 % better than the MPICH original rendezvous implementation.

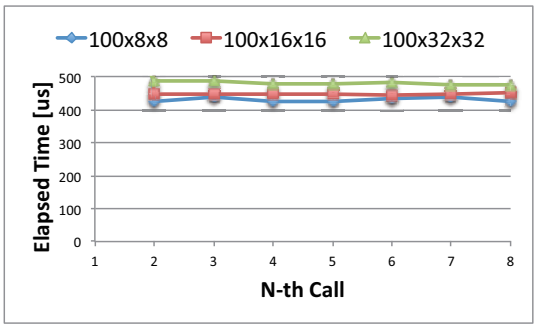


Figure 2 MPICH default implementation

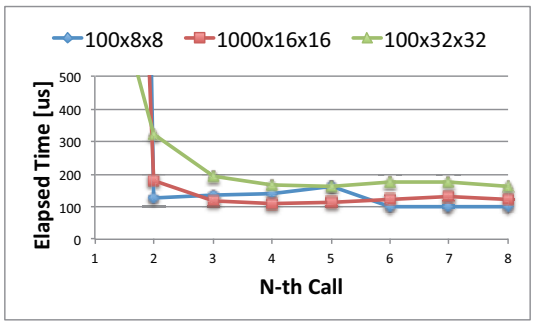


Figure 3 Cached-Multi-W implementation

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 the 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 4 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.

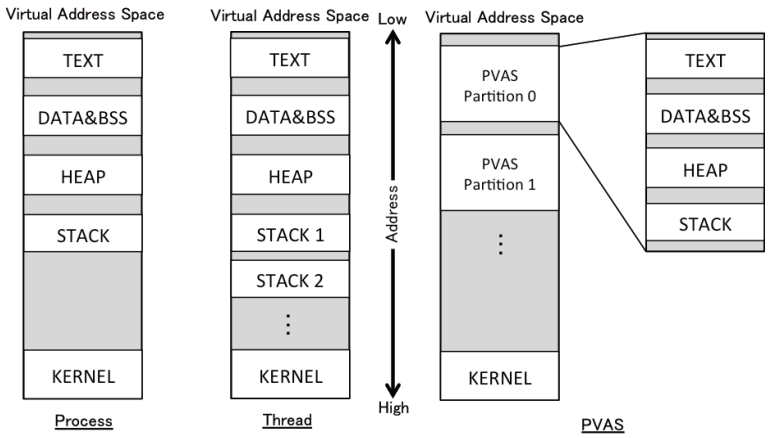


Figure 4 Partitioned Virtual Address Space

In FY2014, we evaluated the PVAS model by implementing a new BTL (a low-level communication layer of OpenMPI) to utilize the advantage of PVAS. In this implementation, the rendezvous protocol is optimized so that only one memory copy operation takes place. Contrastingly, in the current implementation of intra-node communication of OpenMPI, two memory copies must be involved to transfer a message. Figure 5 show the NPB performance comparison of the conventional sm BTL (BTL for shared memory) and our optimized PVAS BTL using the rendezvous protocol. The advantage of PVAS is not only to reduce the number of memory copies, but also to reduce the memory for page tables to map physical memory. In an all-to-all communication, for example, all processes in a node communicate with each other. This results in to map memory regions in $O(N^2)$ and to have $O(N^2)$ page table entries. Figure 6 shows the comparison of all-to-all memory consumption between sm BTL and PVAS BTL. As shown in this graph, conventional sm BTLs consumes memory $O(N^2)$, however, PVAS BTL consumes memory in $O(N)$.

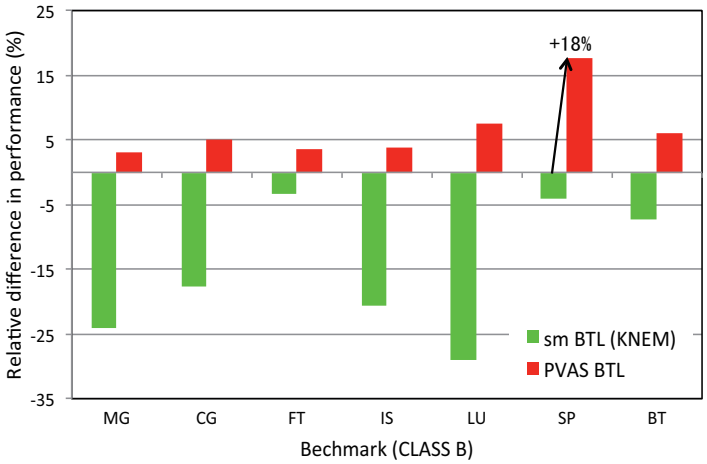


Figure 5 NPB Performance between sm BTL and PVAS BTL (Xeon Phi)

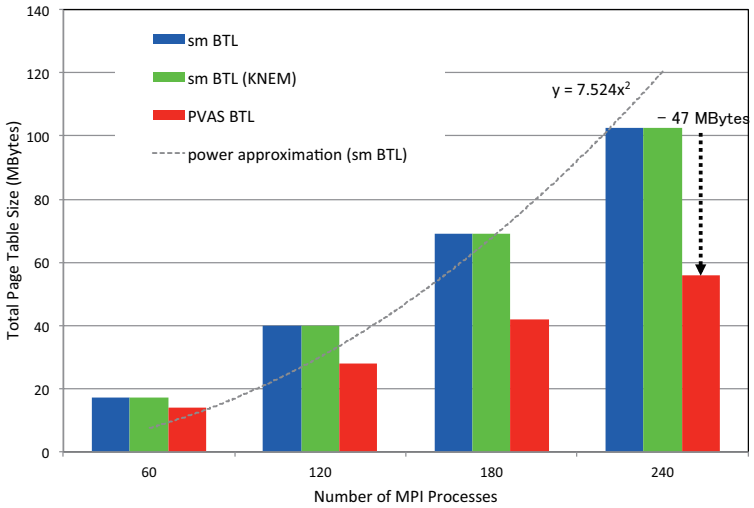


Figure 6 Alltoall Memory Consumption Comparison between sm BTLs and PVAS BTL (Xeon Phi)

3.3. Fault Resilience

With the increasing fault rate on high-end supercomputers, the topic of fault tolerance has been gathering attention. To cope with this situation, various fault-tolerance techniques are under investigation; these include user-level, algorithm-based fault-tolerance techniques and parallel execution environments that enable jobs to continue following node failure. Even with these techniques, some programs that have static load balancing, such as stencil computation, may underperform after a failure recovery. Even when spare nodes are present, they are not always substituted for failed nodes in an effective way.

There are some questions of how spare nodes should be allocated, how to substitute them for faulty nodes, and how much the communication performance is affected by such a substitution. The third question stems from the modification of the rank mapping by node substitutions, which can incur additional message collisions. In a stencil computation, rank mapping is done in a straightforward way on a Cartesian network without incurring any message collisions. However, once a substitution has occurred, the node-rank mapping may be destroyed. Therefore, these questions must be answered in a way that minimizes the degradation of communication performance.

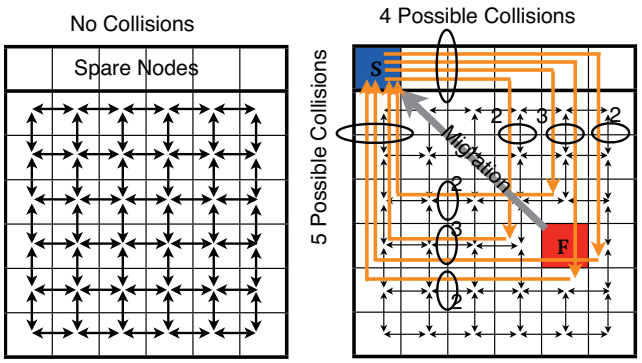


Figure 7 Message collisions by substituting a failed node (5P-stencil)

In FY2014, several spare-node allocation and node-substitution methods were studied, analyzed, and compared in terms of communication performance following the substitution. Three node substitution methods, 0D sliding, 1D sliding and 2D sliding are proposed (Figure 8).

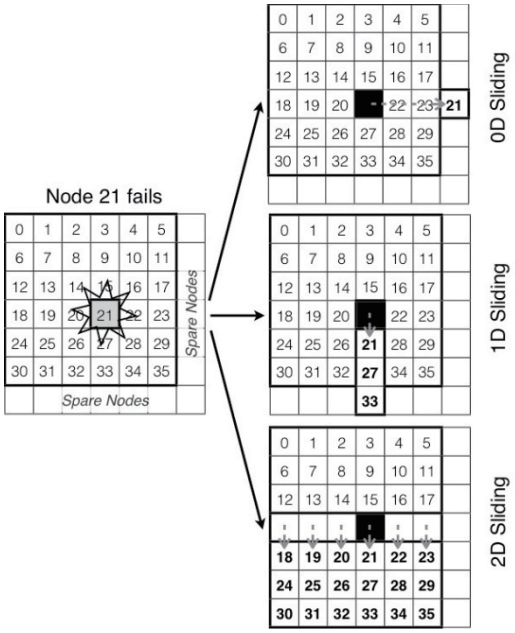


Figure 8 Proposed Three Failed Node Substitution Methods

It was revealed that when a failure occurs, the point-to-point (P2P) communication performance on the K computer can be slowed by a factor of three (Figure 9). On BG/Q, P2P performance can be slowed by a factor of five (Figure 10).

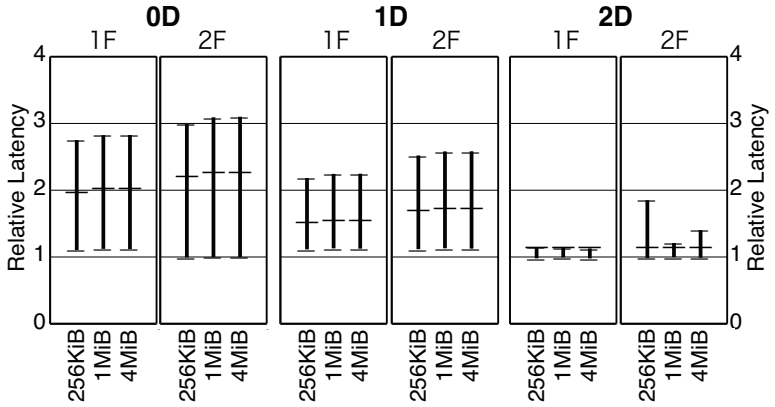


Figure 9 P2P Performance Degradation by Using Spare Node(s) – the K computer

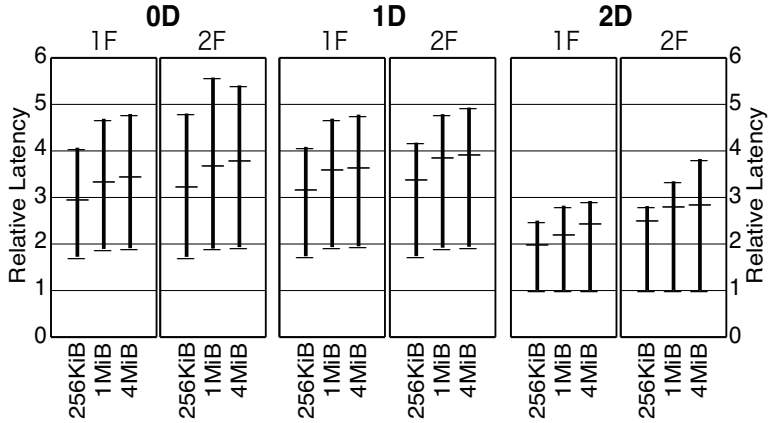


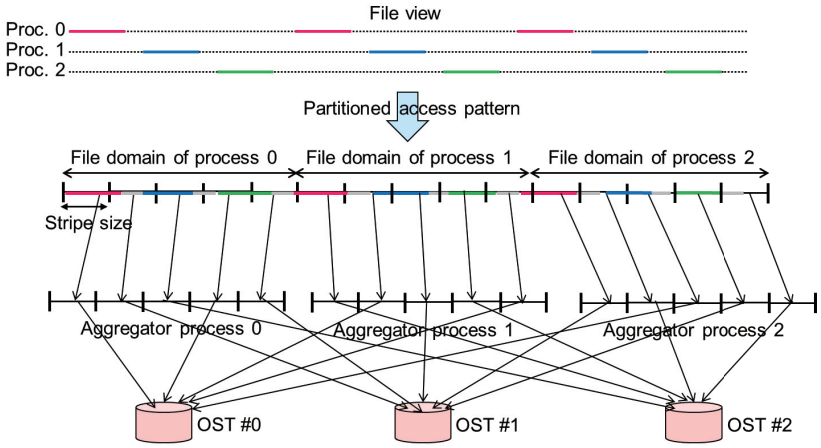
Figure 10 P2P Performance Degradation by Using Spare Node(s) - JUQUEEN (BG/Q)

3.3. Scalable MPI-IO Using Affinity-Aware Aggregation

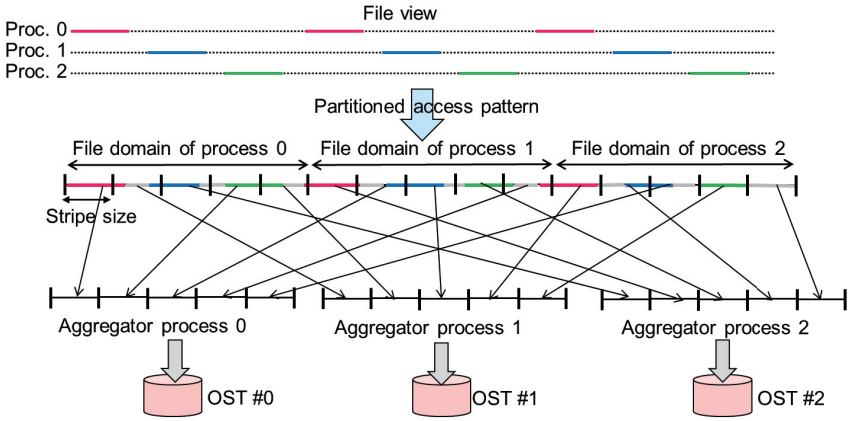
A commonly used MPI-IO library named ROMIO has the two-phase I/O (TP-IO) scheme to improve collective I/O performance for non-contiguous accesses. This research is addressing to optimize TP-IO implementation for further I/O performance improvements than the original one.

In the FY2014, ROMIO in the MPI library on the K computer has been arranged to have (1) affinity-aware data aggregation scheme and (2) I/O throttling approach.

Firstly, we focused to optimize data aggregation scheme. Figure 11 shows I/O flow of TP-IO in the original and optimized ROMIO implementation on the K computer.



(a) Original data aggregation scheme

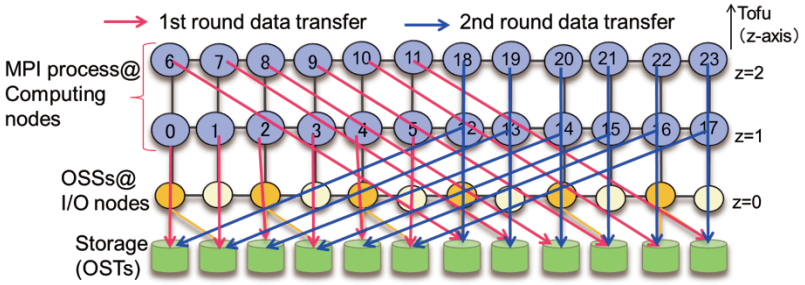


(b) Optimized data aggregation scheme

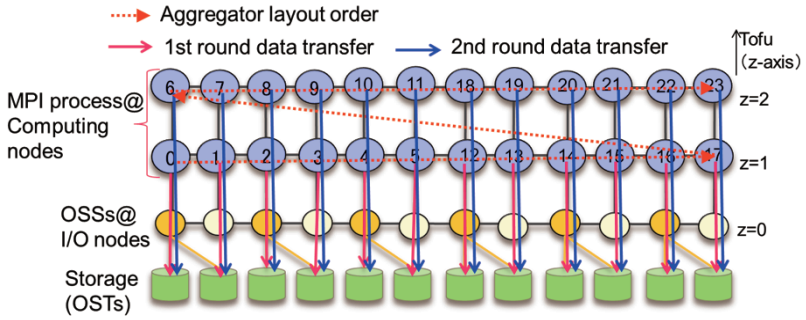
Figure 11 Original and optimized data aggregations in collective write operations

This figure depicts data flow from three MPI processes with the same number of aggregator processes. Figure 11 (a) illustrates TP-IO data flow done in the original implementation on the K computer. In this case, data stream from aggregators are going to each Object Storage Target (OST) of the FEFS file system. As a result, network contention occurs in such data transfer pattern. While in Figure 11 (b) that we adopted based on the similar optimization done for a Lustre file system, each aggregator collects data from every MPI process in order to form striped data layout. Therefore every aggregator just writes collected data to the target OST only, and network contention can be alleviated.

Furthermore, we have focused to have aggregator process layout which suits to the Tofu interconnect configuration of the K computer. Figure 12 shows examples of aggregator process layout and data transfer with striping-oriented aggregation only and with both striping-oriented aggregation and affinity-aware aggregator assignment.



(a) Striping-oriented only (default)



(b) Both striping-oriented & affinity-aware aggregator layout

Figure 12 Aggregator layout and data flow in TP-IO with 2x3x4 process layout

In this figure, data transfers in the first and second rounds of striping accesses on an FEFS file system are illustrated as a simple example. Numbers in circles stand for MPI rank. Since aggregator layout of the former case is based on MPI rank ascending order from zero, network contention or unbalanced network utilization may happen if the aggregator layout does not suit to FEFS's striping layout. On the other hand, the latter case adopts new aggregation layout whose order is independent of user's process layout. The new scheme implemented in a ROMIO library layer checks a 6-D position information, and arranges new groups consisting of MPI processes which are on the same Tofu z-axis. The new scheme finally deploys aggregator task to each MPI process in a round-robin manner crossing Tofu z-axis in order to form FEFS striping layout-aware aggregator layout as shown in Figure 12 (b). As a result, we can eliminate network contention or unbalanced network utilization remarked in Figure 12 (a).

Secondly, I/O throttling was adopted in the above optimized TP-IO implementation. According to previous study about POSIX-I/O on the FEFS file system done in our team, I/O throttling approach succeeded to improve I/O performance. Along with this approach, we implemented a function to control the number of I/O requests generated from computing nodes to a target OST of an FEFS file system in the ROMIO library. Here the I/O request generation is aligned to data access layout on each OST not to have unnecessary file seek operations. Since TP-IO carries out data exchange

phases between file read and write phases in a read-modify-write manner, we also implemented step-by-step data exchanges aligned to the I/O throttling scheme for further improvements. Thus MPI process that generates an I/O request can go to the next data exchange phase not to have a long waiting time for a forthcoming data exchange phase.

Performance evaluation was carried out using computing nodes ranged from 192 to 3,072 nodes. I/O performance evaluation was done by using the HPIO benchmark with non-contiguous access patterns on a local file system of the FEFS on the K computer. The number of nodes was arranged not to have any interference from other users' applications. In the K computer case, we specified the number of nodes in a 3-D manner node allocation, where we chose the following five patterns; 2x3x32, 4x3x32, 8x3x32, 8x6x32, and 8x12x32. We deployed one MPI process per one computing node, thus the number of MPI processes was the same with that of used computing nodes. Figure 13 shows I/O throughput values relative to the number of MPI processes.

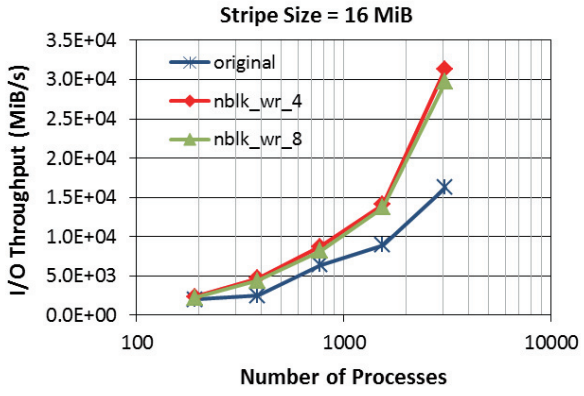


Figure 13 I/O throughput of Collective write

In this evaluation, we examined 4 and 8 for the number of I/O requests in the I/O throttling scheme indicated by "nblk_wr_4" and "nblk_wr_8", respectively in addition to the original implementation indicated by "original." The I/O throttling scheme with affinity-aware aggregation ("nblk_wr_4" and "nblk_wr_8") outperformed the original one and performed higher scalability. We have already observed that the number of I/O requests with 4 or 8 performed the best, but we have not realized why the numbers were the best at this moment. Examinations of properties of the I/O throttling scheme is our future work.

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.

In FY2012-2013, we developed parallel software running on the K computer to analyze images obtained by a light source, SACLA. The developed software consists of two components as shown in Figure 14. The first component is to select the representative images by a classic clustering computation. Thus, all images must be compared with all others. The second component is to classify the rest of images into the representative images. In this stage, we need to calculate for all possible combinations of representative images and rest of images.

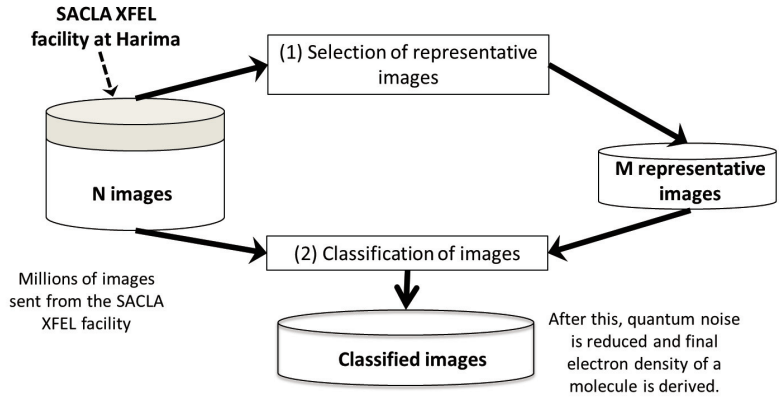
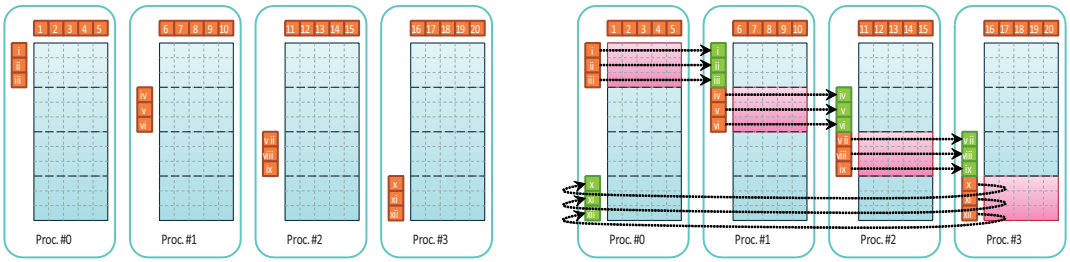
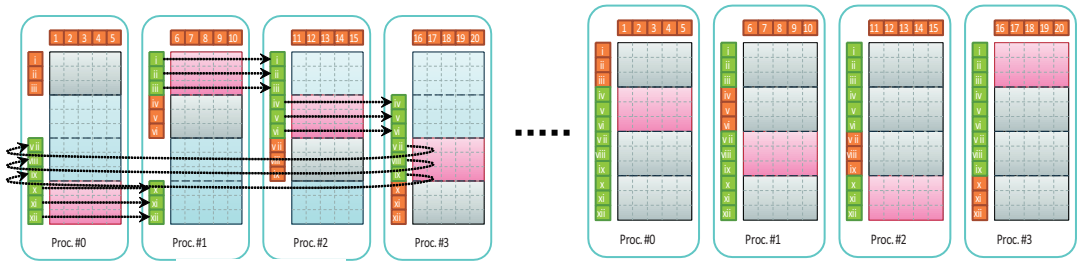


Figure 14 Block diagram of the procedure running on the K computer

In order to realize effective parallelization, the developed software keeps load balance between processes and reduces file input time by minimizing total size of the input from storage. Figure 15 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 15 are images which are read from storage, and the greens are transferred from the neighbor process. The calculation is finished at N_p step, where N_p is number of processes.



Initial State　　Step 1



Step 2 Last Step (Step N_p, N_p is # of procs)

Figure 15 Calculation workflow for classification of images

In FY2014, based on the developed software, we designed a new framework, named *pCarp*, that describes any possible combination of two records in a dataset processed by all participating processes. This parallel processing is used not only our target application, but also used to analyze gene sequencing data, images obtained by electron microscopes, and so on. The framework users do not need to write any parallel program, but write just sequential program. All parallelizing tasks are performed by *pCarp*.

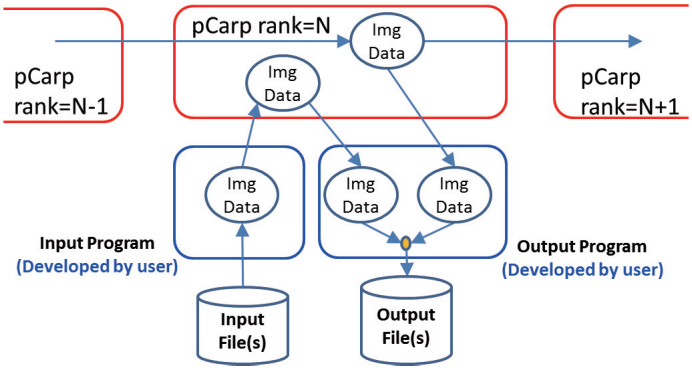


Figure 16 Decoupling Architecture of *pCarp*

```
main( argc, argv ) {

  ReadDataFile( data, size, &datacnt );

  for( i=0; i<datacnt; i++ ){
    carp_put_datasize( size[i] );
    carp_write( &data[i], size[i] );
  }
}
```

Input program

```
main( argc, argv ) {
  for( ... ) {
    carp_get_datasize( &size0 );
    carp_read( &data0, size0 );
    carp_get_datasize( &size1 );
    carp_read( &data1, size1 );
    result = kernel_code( data0, data1 );
    OutputData( result );
  }
}
```

Output program

Figure 17 Code skeletons of the input and output processes

Figure 16 shows the decoupled architecture of the image analyzing software for XFEL using *pCarp*. Each MPI process (*pCarp* process) creates two sub-processes by using the POSIX popen I/O

function, one to read a file and the other to process two data records and output its result to a file. Figure 17 shows the code skeletons of the input and output processes in Figure 16, the function having bold face names are the function provided by the *pCarp* framework. The input sub-process reads a file and passes read records to the parent *pCarp* process. In the *pCarp* process, records are preserved in memory and sent to its neighbor process as shown in Figure 15. The output sub-process reads two records from parent *pCarp* process and then computes those records. Finally its result is output. This procedure is repeated until the all data of the desired all-to-all computation is done. In those input and output programs, there is no need of calling the complex MPI functions at all.

In the evaluation of current prototype of *pCarp*, the execution time is much larger than the original program depending on the data size. The most of the additional time of *pCarp* comes from the pipe transmission. Improving this data transmission performance is our future work.

3.5. File Composition Library

We have been developing a user-level file I/O library, called file composition library, to reduce the heavy load on both the metadata and object storage servers of a parallel file system. The file composition library is assumed to use the SPMD (Single Program Multiple Data) execution model. In other words, it is assumed that all processes access each own file and issue the same I/O operations. The heavy load in the metadata is caused by issuing file open/create/close operations by a large number of processes. The file composition library gathers all files created by a job and make them a single file so that the metadata accesses are reduced. To mitigate the heavy load in the object storage, the file composition library limits the number of processes accessing a parallel file server simultaneously. In FY 2014, based on the experiences of developing the file composition library, a new file I/O library, called ftar (Fragmented tar), was designed. Unlike the file composition library, ftar uses the tar format. An ftar file keeps the tar format, but each file may be stored in fragments. Figure 18 shows an example of ftar file in which two files, f1 and f2, are stored in fragments.

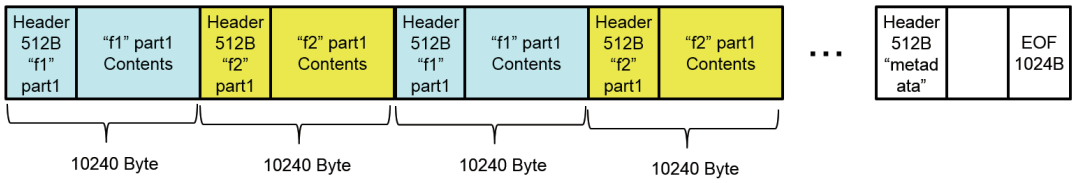


Figure 18 An Example of Ftar format

4. Schedule and Future Plan

- Communication Library

  Cached-Multi-W implementation on MPI_Neighbor_alltoallw primitive will be enhanced and

evaluated. This approach will also be applied to MPICH one-sided implementation using MPI_Put and MPI_Win_fence primitives.

- New Process / Thread Model

  Integratation the proposed task model with the McKernel which is under development by AICS System Software Development team is planned. Also, we are doing a collaborative research with ANL on the User-level process which was developed in last FY2013 to enhance the performance of irregular applications.

- Fault Resilience

  Based on the investigation in FY2014, we will start developing a framework to allow user applications to be fault-resilient easily.

- File I/O

  pCarp will be enhanced and distributed as open source. As mentioned in section 3.4. , the most of overhead of pCarp comes from data transmission using pipe. In order to reduce this overhead, we will try to implement pCarp with shared memory.

  The scalable MPI-IO will be adapted to the FEFS file system used in the K computer. Although the scalable MPI-IO implementation manages data exchanges in the two-phase I/O optimization using MPI_Isend and MPI_Irecv among MPI processes, we will try to apply MPI_Alltoallv for data exchanges as an alternative implementation for further performance improvement. I/O throttling scheme will be also examined in the collective data exchanges.

  Ftar will be developed and distributed as open source.

5. Publication, Presentation and Deliverables

(1) Journal Papers

1. 島田 明男, 堀 敦史, 石川 裕, 新しいタスクモデルによるメニーコア環境に適したMPI ノード内通信の実装, 情報処理学会論文誌, 情報処理学会, volume 56, 2015.

(2) Conference Papers

1. Yuichi Tsujita, Atsushi Hori, Yutaka Ishikawa: “Locality-Aware Process Mapping for High Performance Collective MPI-IO on FEFS with Tofu Interconnect,” In Proceedings of the 21th European MPI User’s Group Meeting, Workshop on Challenges in Data-Centric Computing, ACM, 2014.
2. Yuichi Tsujita, Atsushi Hori, Yutaka Ishikawa: "Affinity-Aware Optimization of Multithreaded Two-Phase I/O for High Throughput Collective I/O," In Proceedings of International Conference on High Performance Computing & Simulation, HPCS 2014, IEEE, 2014.
3. Yuichi Tsujita, Kazumi Yoshinaga, Atsushi Hori, Mikiko Sato, Mitaro Namiki, Yutaka

Ishikawa: "Multithreaded Two-Phase I/O: Improving Collective MPI-IO Performance on a Lustre File System," 22nd Euromicro International Conference on Parallel, Distributed, and Network-Based Processing, PDP 2014, 2014.

4. Yuichi Tsujita, Kazumi Yoshinaga, Atsushi Hori, Mikiko Sato, Mitaro Namiki, Yutaka Ishikawa: "Improving Parallel I/O Performance Using Multithreaded Two-Phase I/O with Processor Affinity Management," PPAM 2013 Revised Selected Papers, Lecture Notes in Computer Science, Vol. 8384, Springer, pp. 714-723, 2014.
5. Balazs Gerofi, Akio Shimada, Atsushi Hori, Takagi Masamichi, Yutaka Ishikawa: "CMCP: A Novel Page Replacement Policy for System Level Hierarchical Memory Management on Many-cores," In Proceedings of the 23rd International Symposium on High-performance Parallel and Distributed Computing, ACM, 2014.
6. Mikiko Sato, Go Fukazawa, Akio Shimada, Atsushi Hori, Yutaka Ishikawa, Mitaro Namiki, “Design of Multiple PVAS on InfiniBand Cluster System Consisting of Many-core and Multi-core,” In Proceedings of the 21st European MPI Users' Group Meeting, ACM, 2014.
7. Atsushi Hori, Kazumi Yoshinaga, Atsushi Tokuhisa, Yasumasa Joti, Kensuke Okada, Takashi Sugimoto, Mitsuhiro Yamaga, Takaki Hatsui, Makina Yabashi, Yuji Sugita, Yutaka Ishikawa, Nobuhiro Go, “Decoupling Architecture for All-to-all Computation,” In Proceedings of the 21st European MPI Users' Group Meeting, ACM, 2014.
8. 畑中正行, 堀敦史, 石川裕, 京 Tofu における MPI-3.0 隣接集団通信の実装と評価, 情報処理学会, プログラミング 7(5), 2014.
9. 山口 訓央, 高木 将通, 畑中 正行, 堀 敦史, 石川 裕, HPC 向け高可搬通信ライブラリの設計と評価, 情報処理学会, 2014-HPC-145, No. 15, 2014.
10. 島田 明男, 堀 敦史, 石川 裕, 新しいタスクモデルによる MPI ノード内通信の高性能化, 情報処理学会, 2014-OS-130, No. 18, 2014.
11. 吉永一美,亀山豊久,堀敦史,石川裕,エクサスケールでの耐故障性実現に向けた代替ノード配置による通信性能の評価, 情報処理学会, 2014-HPC-144, No.16, 2014.
12. 吉永一美,亀山豊久,畑中正行,堀敦史,石川裕, 代替ノード利用手法による耐故障性実現に向けた通信性能の評価と検討, 情報処理学会, 2014-HPC-145, No.6, 2014.
13. 吉永一美,亀山豊久,堀敦史,石川裕,予備ノードを利用した故障後の実行継続手法の検討と評価, 情報処理学会, 2014-HPC-147, No.21, 2014.
14. 畑中正行, 堀敦史, 石川裕, 京 Tofu における隣接集団通信の袖通信最適化, 情報処理学会, 2015-HPC-148(35), 2015.
15. 辻田　祐一，堀　敦史，石川　裕，FEFS におけるストライピング処理を考慮した集団型 MPI-IO の実装，情報処理学会，2014-HPC-145，No. 35, 2014.
16. 辻田　祐一，堀　敦史，石川　裕，集団型 MPI-IO の高速化に向けた I/O リクエスト発行方式の最適化，情報処理学会,2014-HPC-146，No. 17, 2014.

17. User-level Process towards Exascale Systems (Akio Shimada, Atsushi Hori, Yutaka Ishikawa, Pavan Balaji), In 情報処理学会研究報告. 計算機アーキテクチャ研究会報告, 一般社団法人情報処理学会, volume 2014, 2014.
18. メニーコアクラスタにおけるジョブ間の性能干渉について (堀 敦史, 亀山 豊久, 並木 美太郎, 石川 裕), 情報処理学会研究報告. HPC 研究会報告, 一般社団法人情報処理学会, volume 2014, 2014.

(3) Invited Talks

(4) Posters and presentations

1. Akio Shimada, Atsushi Hori, Yutaka Ishikawa, “Eliminating Costs for Crossing Process Boundary from MPI Intra-node Communication,” In Proceedings of the 21st European MPI Users' Group Meeting, ACM, 2014.

(5) Patents and Deliverables

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

1. PRDMA (for the K computer)
2. GDB for McKernel
3. PVAS, M-PVAS and Agent (for the x86 and Xeon Phi CPUs)
4. sCarp and pCarp (for the K computer, FX10s and Linux clusters)

Programming Environment Research Team

1. Team members

Mitsuhisa Sato (Team Leader)
Hitoshi Murai (Research Scientist)
Miwako Tsuji (Research Scientist)
Masahiro Nakao (Research Scientist)
Hidetoshi Iwashita (Research Associate)
Makoto Ishihara (Agency Staff)
Masahiro Yasugi (Senior Visiting Researcher)
Hitoshi Sakagami (Senior Visiting Researcher)
Brian Wylie (Visiting Researcher)
Christian Feld (Visiting Researcher)
Kengo Nakajima (Senior Visiting Researcher)
Tomoko Nakashima (Assistant)

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 conduct 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 2014FY, in order to archive these objectives above, we carried out the following researches:

1) We are working on the development and improvement of XcalableMP (XMP) programming languages. XcalableMP is a directive-based language extension, designed by XcalableMP Specification Working Group (XMP Spec WG) including some members from our team as a community effort in Japan. It allows users to develop parallel programs for distributed memory systems easily and to tune the performance by having minimal and simple notations. In this year, we have implemented Coarray functions in Fortran and C using one-sided communication supported efficiently by the K computer.
2) As an extension of XcalableMP to exascale computing, we are proposing a new programming model, XcalableACC, for emerging accelerator clusters, by integrating XcalableMP and OpenACC. We are working on the language design and the compiler development of XcalableACC. We have submitted the results of XcalableACC and XcalableMP to SC14 HPCC class 2 competition, and awarded "HPCC Class2 Performance Award". This research is funded

by JST CREST project on “post-petascale computing”.

3) As a follow-up of Japan-France project FP3C, "Framework and Programming for Post Petascale Computing" (2010-2013), and have been investigated fault tolerance mechanism for a multiple SPMD programming environment, FP2C (Framework for Post-Petascale Computing), developed in FP3C project. This work focuses on the technique of fault tolerance on workflow by replaying faulted tasks.
4) As a study on performance evaluation of the K computer, we are working on HPGMG, a new HPC benchmark program developed by Lawrence Berkeley National Laboratory (LBNL). For large-scale parallel applications, we continue the design of parallel communication library to support the communication between a set of multiple processes in Multiple processes Multiple Data (MPMD), named MPMPI library.
5) 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 (Oct. 24)
- FOCUS seminar on XMP (Sep. 18, Dec. 18)

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

3. Research Results and Achievements

3.1. Development of an XcalableMP compiler

We are developing Omni XcalableMP that is an open-source XcalableMP compiler, in cooperation with the university of Tsukuba. The latest version 0.9.1 has been released in April, 2015

3.1.1. Coarray Fortran and C

Coarray Fortran (CAF) is a parallel language that is a language extension of Fortran. Since it was accepted as a part of the latest Fortran standard Fortran2008, it is expected to be popular gradually. CAF is a lower-level language than XMP we have been developing and seems to be suitable for fine performance tuning. Therefore, we expect CAF not to be a competitor but to be a complementary to XMP.

This year we started to develop Coarray features into our XMP translator. In general, it is not easy to develop such low-level language as a translator, a source-to-source compiler. The gorl of

development is both functionality to be worth using real-world applications and high performance comparable with MPI library. And we will extend the experience of CAF also into C language.

Now we have developed major features of CAF1.0 specification such as declaration of coarray variables, reference and definition of remote coarray data objects, and dynamic allocation and explicit and automatic deallocation. During the development, we encountered and solved some issues as follows.

- Memory allocation of a coarray variable brings inter-node synchronization as a side effect. It had caused overhead cost at the start point of every procedure containing coarray. To move out and aggregate the costs, we developed a new mechanism which works just before the linkage-editor. It scans all object and archive files to be linked, finds coarrays to be allocated and initialized at the runtime, and generates instructions to allocate and initialize them previously before execution of the user program.
- For effective inter-code communication of coarray data, it is required at runtime to detect how long data is contiguous and how the contiguous data appear frequently. We developed a new interface, which has information made from parameters of multi-dimensional subarray data in Fortran language and is easy to detect how contiguous the data at runtime.

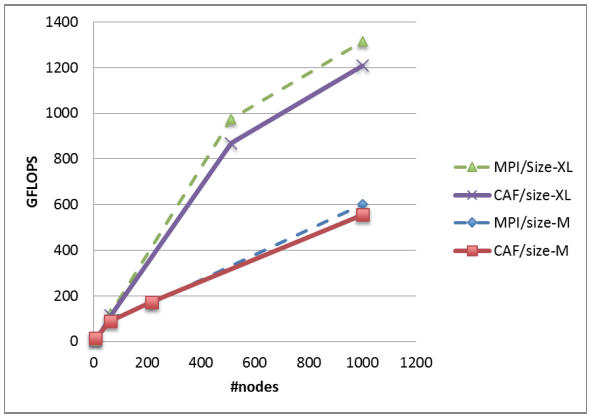


Fig. 1 Comparison of CAF and XMP

We evaluated the current compiler we have developed and concludes that the compiler works correctly with a program written by CAF and the performance is very close to the one of MPI. Fig. 1 shows comparison of CAF and MPI with Himeno benchmark. The MPI program is basically the same as the original and the CAF program was ported from it. In spite of the data size M and XL, the difference of the performance was 10 percent or less. And we still have room for improvement both the compiler and the CAF program.

According to the development and evaluation, we found CAF can be implemented even as a translator with high performance. And the program written in CAF seems much easier than the one of MPI. The latest XMP compiler with the CAF features was released in April 2015.

3.1.2. Evaluation of productivity and performance of XcalableMP

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 High Performance Linpack (HPL), Fast Fourier Transform (FFT), STREAM, and RandomAccess.

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 benchmarks

	HPL	FFT	STREAM	RandomAccess
XcalableMP	313	204	69	253
Reference	8,800	787	329	938

All benchmarks were compiled by using the Omni compiler 0.9.0-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. 2 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 SC14 HPC Challenge Benchmark Class2 Competition, and we have awarded the HPC Challenge Class 2 Best Performance Award.

Last year, we had implemented the HPCC benchmarks. This year, we have tuned the Omni Compiler for the K computer and algorithms of HPCC benchmarks. Fig. 3 shows the comparison between implementations of last year and this year.

While the SLOCs of this year are almost the same as those of last year, the performance of this year are better than those of last year.

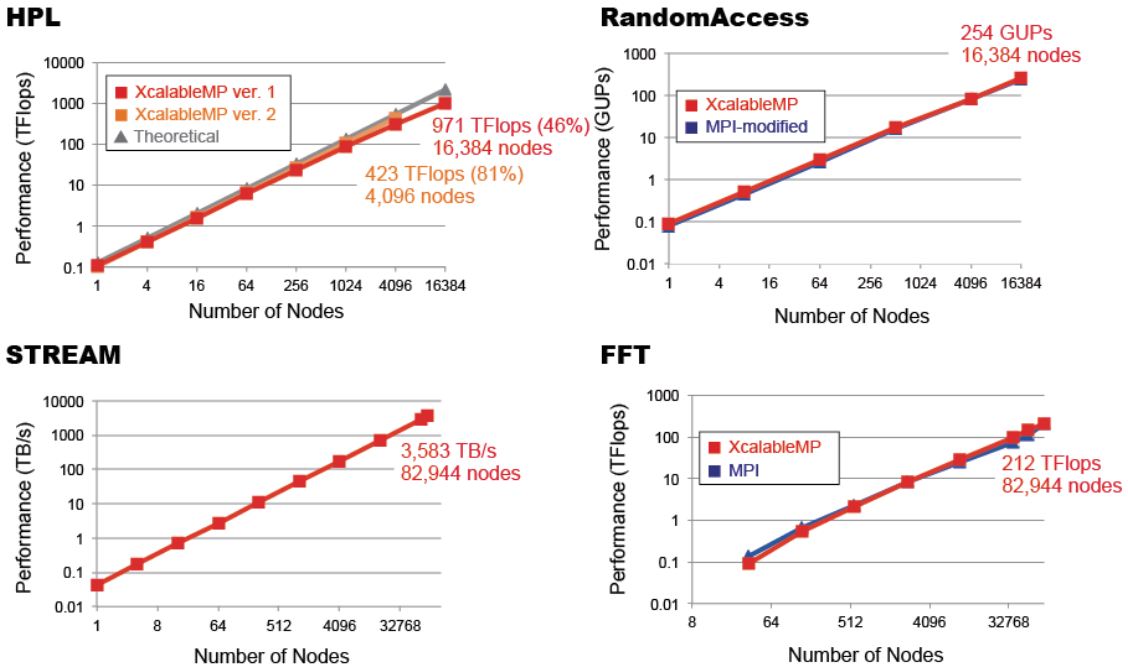


Fig. 2 Performance results of HPCC benchmarks

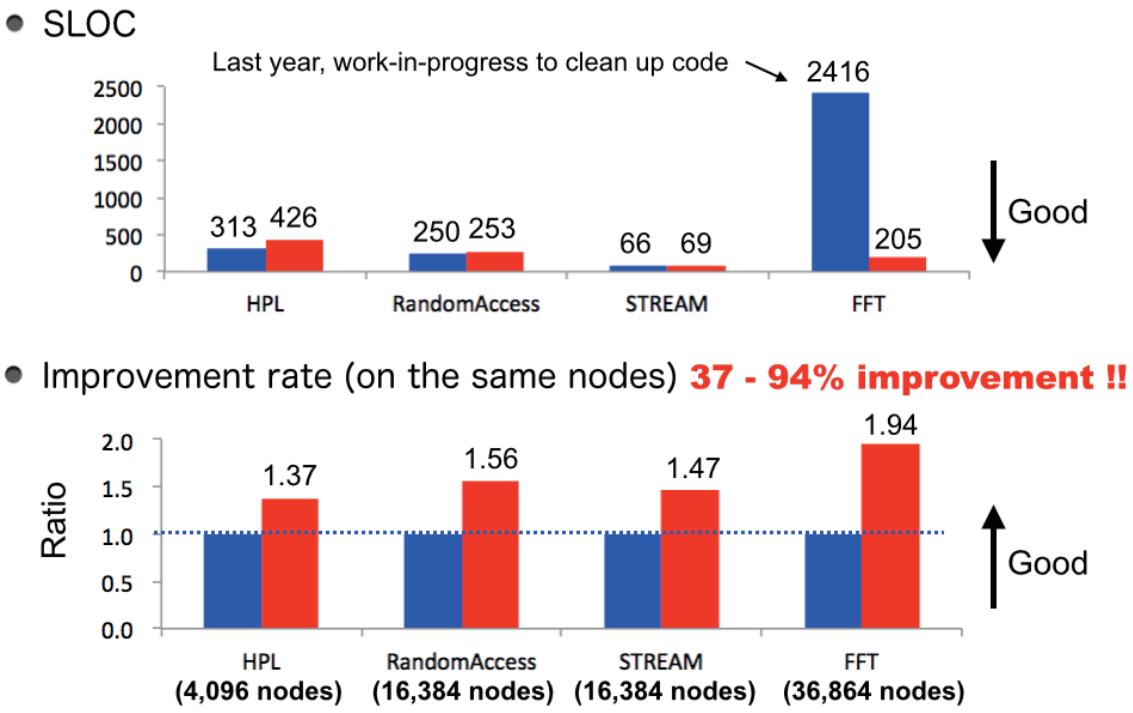


Fig. 3 Comparison between last year and this year

3.2. Multiple SPMD programming environment for fault tolerance

To develop a multiple SPMD programming environment supporting fault tolerance feature, we have extended middleware and developed the prototype environment by incorporating the middleware to the multiple SPMD programming environment.

During recent years, we have developed a multiple SMPD programming environment called FP2C (Framework for Post-Petascale Computing) with our domestic and international collaborators such as University of Tsukuba, University of Versailles, Maison de la Simulation etc… The FP2C combines several programing methodologies such as workflow, distributed parallel, shared memory and allows programmers to make hierarchical programs across multiple architectural levels such as intra-node, inter-node and inter-cluster. In FP2C, a workflow application is executed by YML --- a development and execution environment for a workflow --- and each task in the workflow can be distributed parallel program described XMP, MPI and so on.

YML workflow scheduler uses different middlewares for different programming environments. Especially, in clusters and supercomputers, it adopts OmniRPC-MPI, which is an extension of OmniRPC (Remote Procedure call library) for parallel remote programs. To realize fault tolerance, we have extended OmniRPC-MPI to OmniRPC-MPI-FT by implementing heartbeat messages. Moreover, FJMPI, which is MPI library provided by Fujitsu to realize "safe" communication between two communicators.

Although the OmniRPC-MPI had been developed for FP2C, it can work as an independent RPC library. Therefore, we have implemented the OpenFMO, which is one of fragment molecular orbital methods, with the OmniRPC-MPI-FT. According to the experimental results, while the overhead of the heartbeat messages seems to be ignorable, FJMPI is not efficient.

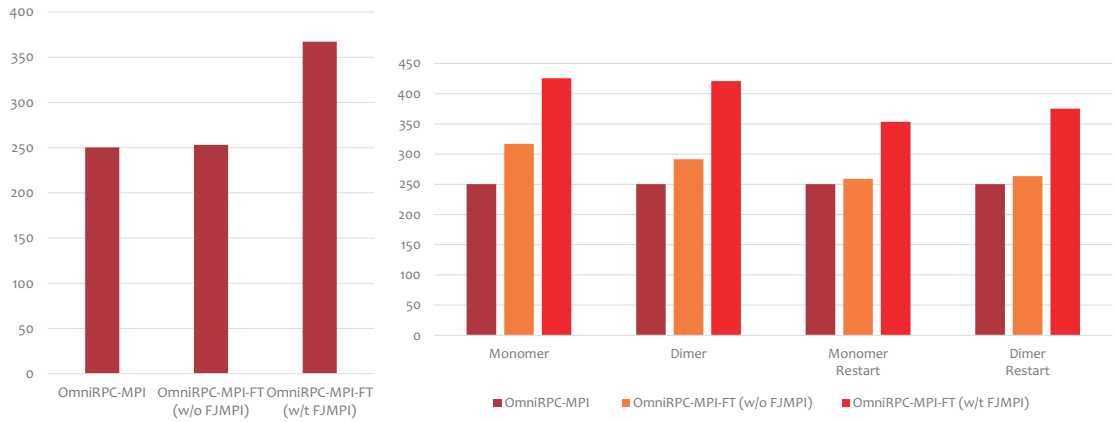


Fig. 4 elapse time.

We have also incorporated the OmniRPC-MPI-FT to the FP2C and improve the algorithm of our workflow scheduler in order to realize automatic fault detection and recovery. FJMPI "safe" communication had not been adopted. We have considered a "task-wise" strategy, in which if the scheduler detects an error in a task, it retries the task until successful completion. We have performed computational experiments with a block Gauss Jordan application and confirmed that

- If FP2C have several tasks simultaneously, it can recover error and complete the whole application.
- The overheads of heartbeat messages and fault recovery are acceptable.

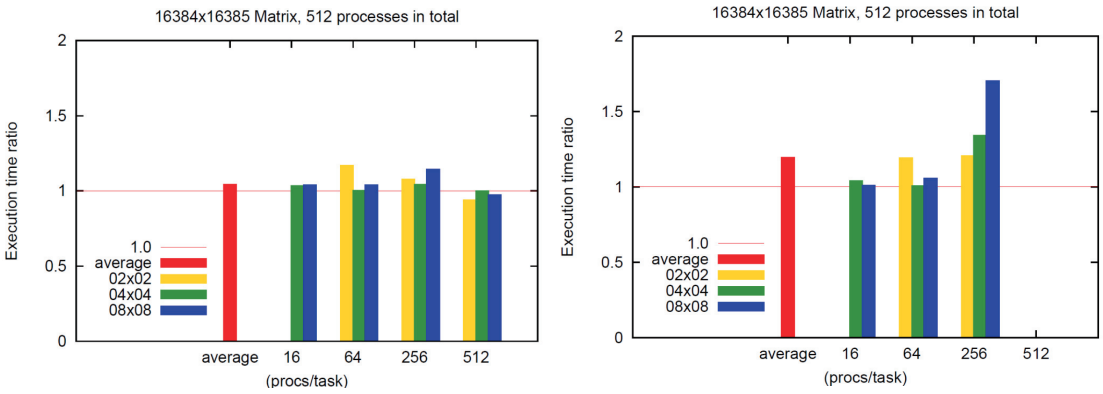


Fig. 5 The ratio of execution time without error(left) and with error(right)

3.3. XcalableMP Extension for Accelerator Clusters

We are designing a new programming model and developing its compiler for emerging accelerator clusters. Specifically, we target 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 technology for communication between accelerators. This research is supported by CREST, JST.

3.3.1. XcalableACC language

In order to improve productivity of applications using TCA and accelerators, we have developed a new programming model XcalableACC (XACC), which is a combination of XcalableMP and OpenACC, enhanced by features for controlling multi-devices and direct communication between devices (Table 2)

Table 2 XcalableACC directives

XMP directives	distributed-memory parallelism among nodes
OpenACC directives	parallelism inside a device
XACC extensions	parallelism among devices and direct communication

Fig. 6 illustrates the basic concept of XACC.

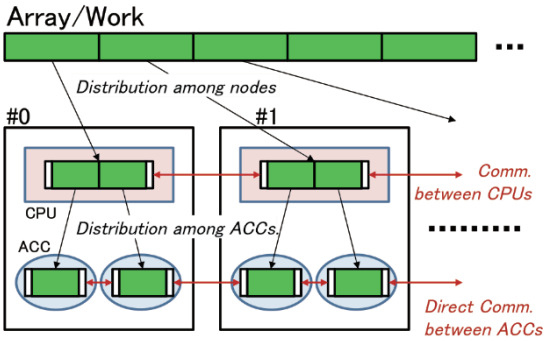


Fig. 6 Execution Model of XACC for data distribution, offloading, and communication

The XACC extensions for parallelism among devices and direct communication include the following clauses and directives.

- acc clause, which specifies which instance of the data (on CPU or ACCs) is to be communicated;
- device directive, which declares an *XACC device* that may be a set of ACCs;
- on_device clause, which specifies the target ACC of OpenACC directives;
- layout clause, which specifies data/work mapping onto an XACC device;
- shadow clause, which specifies the stencil area of a distribute array; and
- barrier_device directive, which specifies a barrier among devices.

Programmers could write their programs for ACC cluseters using XACC with less dificullty than using the de facto approach, the combination of MPI and CUDA. An example code of XACC is given in Fig. 7

```
void foo(){

#pragma xmp nodes p(4)
#pragma acc device d(*)

#pragma xmp template t(0:99)
#pragma xmp distribute t(block) onto p

  float a[100][100];
#pragma xmp align a[i][*] with t(i)
#pragma xmp shadow a[1:1][0]
#pragma acc declare copy(a) layout([*][block]) shadow([0][1:1]) on_device(d)

#pragma xmp reflect (a) acc

#pragma xmp loop (i) on t(i)
  for (int i = 0; i < 100; i++){
#pragma acc parallel loop layout(a[*][j+1]) on_device(d)
    for (int j = 0; j < 99; j++){
      a[i][j+1] = 1;
    }
  }

}
```

Fig. 7 Example code of XACC

3.3.2. Omni XcalableACC Compiler

We are also developing a compiler for XACC, named Omni XcalableACC, in collaboration with the university of Tsukuba. It works as an extended function of the Omni XcalableMP compiler (Fig. 8).

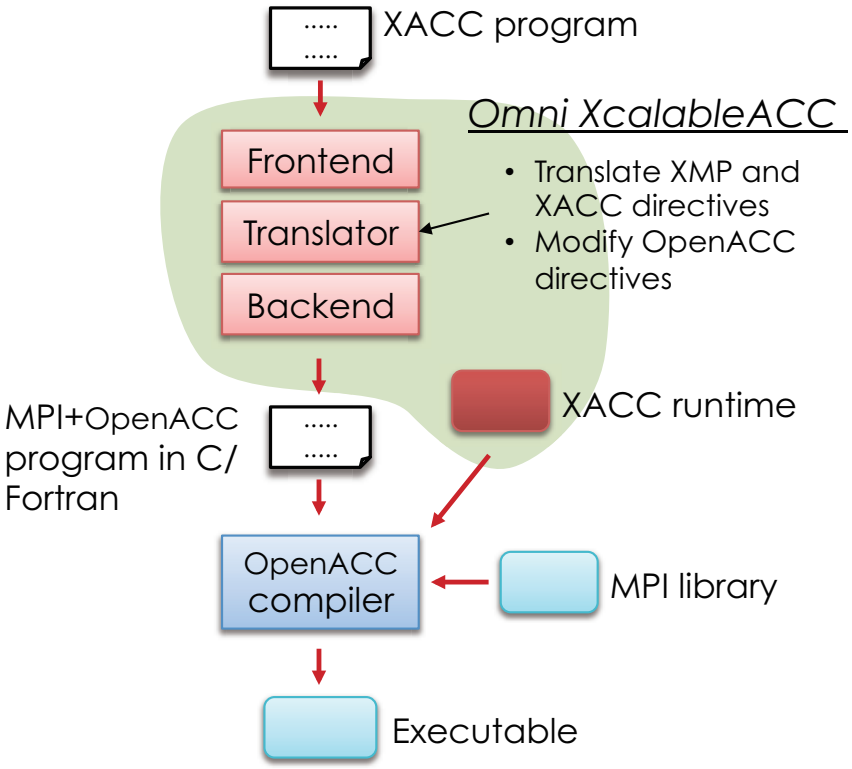


Fig. 8 Configuration of Omni XcalableACC

In this year, we have implemented basic functions of XACC, which include the feature of stencil communication (the reflect directive) based on TCA.

We parallelized the HIMENO benchmark, which is a typical stencil code, with Omni XACC and evaluated its performance on HA-PACS/TCA, which is an accelerator cluster based on the TCA architecture located at Center for Computational Sciences, University of Tsukuba. Fig. 9 and Table 3 show that, using XACC, programmers could enjoy both higher performance and productivity than using the normal means of OpenACC+MPI.

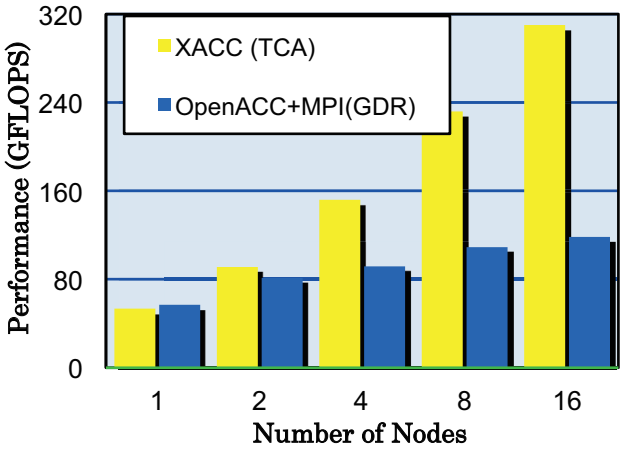


Fig. 9 Performance on HA-PACS/TCA

Table 3 Comparison of Source Lines of Code

	total	XMP	OpenACC	others
XACC	213	28	9	176
OpenACC + MPI	488	-	15	473

Other achievements in this year include prototyping the features of multi-devices and communication on a hybrid network of Infiniband and TCA.

3.3. Evaluation of HPGMG and HPCG

HPGMG is a new HPC benchmark program developed by Lawrence Berkeley National Laboratory (LBNL). Current most famous HPC benchmark program is High Performance Linpack (HPL), which is adopted by TOP500 (http://www.top500.org). HPL has a weakness of very long execution time for large-scale parallel computers because the execution time is proportional to the problem size. HPGMG is developed as an alternative to HPL.

HPCG (https://software.sandia.gov/hpcg/) has also the similar purpose. Both HPGMG and HPCG use iterative solvers based on the multigrid method: a finite-element solver (HPGMG-FE) and a finite-volume solver (HPGMG-FV) in HPGMG, and a symmetric Gauss-Seidel preconditioned conjugate gradient solver in HPCG.

Our team started cooperation in evaluating HPGMG-FV on Apr. 2014. We adjusted tuning parameters of HPGMG-FV for the K computer and measured its weak scaling performance.. As the result, we achieved the first rank of performance in Mar. 2015, as shown at the website of LBNL

(http://crd.lbl.gov/departments/computer-science/performance-and-algorithms-research/research/hpgmg/). Moreover we investigated performance characteristics of HPGMG-FV and HPCG using the profiler of the K computer.

Table 4 shows the weak scaling performance, the ratio of GFLOPS to the peak, and the SIMD occupation rate, as well as the performance without SIMD for comparison. Table 5 shows performance characteristics of HPCG optimized by RIKEN AICS software development team.

Table 4 Weak scaling performance of HPGMG on the K computer

Number of nodes	1	8	64	512	4096	32768	82944
DOF/s (SIMD)	3.99E+07	3.06E+08	2.40E+09	1.89E+10	1.50E+11	1.14E+12	2.83E+12
GFLOPS/Peak(%)	10.3107	9.8652	9.6761	9.5043	9.3916	8.8612	8.6821
SIMD rate(%)	61.5931	61.3401	61.9923	61.1174	61.0208	60.5174	60.425
DOF/s(NOSIMD)	3.88E+07	2.96E+08	2.33E+09	1.84E+10	1.46E+11	1.10E+12	

DOF/s: Degree of Freedom per Second

Table 5 Weak scaling performance of HPCG on the K computer

Number of nodes	1	8	64	512	4096
GFLOPS/Peak(%)	4.37229	4.2616	4.1228	4.10028	4.10913
SIMD rate(%)	17.1305	17.0965	17.0283	17.0269	17.0357

The ratio of GFLOPS to the peak and the SIMD occupation rate in Table 4 are different from those in Table 5 because smoothers of HPGMG and HPCG use different methods: chebychev polynomial and Gauss-Seidel, respectively. Currently, for both benchmarks, SIMD instruction have no effect.

4. Schedule and Future Plan

One of important action for XcalableMP project in recent years is to disseminate our XcalableMP to applications users. As in last year, we organized several schools and hands-on, workshop with potential users also in this year. 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.

The programming models for post-petascale will be investigated, including programming models and runtime techniques to support manycore and accelerators such as GPU in large-scale parallel system. XcalableACC is our solution for accelerator-based system, which is to be explored in the

JST CREST project. As the post-K computer will be a large-scale multicore-based system, we will investigate programming models for manycore-based parallel systems including dynamic tasking and load balancing as well as advanced PGAS models for distributed memory systems.

5. Publication, Presentation and Deliverables

(1) Journal Papers

(2) Conference Papers

1. Swann Perarnau, Mitsuhisa Sato: Victim Selection and Distributed Work Stealing Performance: A Case Study. IPDPS 2014: 659-668
2. Masahiro Nakao, Hitoshi Murai, Takenori Shimosaka, Akihiro Tabuchi, Toshihiro Hanawa, Yuetsu Kodama, Taisuke Boku, Mitsuhisa Sato. ``XcalableACC: Extension of XcalableMP PGAS Language using OpenACC for Accelerator Clusters," Workshop on accelerator programming using directives (WACCPD), New Orleans, LA, USA, Nov., 2014.
3. Takenori Shimosaka, Hitoshi Murai, Mitsuhisa Sato, "A Design of a Communication Library between Multiple Sets of MPI Processes for MPMD," 2014 IEEE 17th International Conference on Computational Science and Engineering (CSE), pp.1886,1893, 19-21 Dec. 2014

(3) Invited Talks

1. Hitoshi Murai, “XcalableACC: a PGAS Language for Accelerated Parallel Computers,” JST/CREST International Symposium on Post Petascale System Software, Kobe, Japan, 2014-12-04
2. Mitsuhisa Sato, HPC research and development in Japan - Post T2K and post K project -, EuroMPI/Aisa 2014.

(4) Posters and presentations

1. Miwako Tsuji, FP2C a multi-level programming paradigm, J-F Conference Extreme Performance Computational Science, Apr. 2014
2. Miwako Tsuji,The extension of OmniRPC-MPI toward fault tolerant computation, 1st workshop on middleware for fault tolerant, July. 2014 (in Japanese)
3. Takenori Shimosaka, Hitoshi Murai, Mitsuhisa Sato, "Efficient FFT implementation in XcalableMP". IPSJ SIG Technical Report, 2014-HPC-145, Jul. 2014 (in Japanese)
4. Masahiro Nakao, Hitoshi Murai, Takenori Shimosaka, Akihiro Tabuchi, Toshihiro Hanawa, Yuetsu Kodama, Taisuke Boku, Mitsuhisa Sato. “XcalableACC : An extension of XcalableMP for accelerator cluster system”, 2014-HPC-146(7),1-11, Oct. 2014 (in Japanese).

5. Masahiro Nakao, “Performance result and implementation of HPC Challenge Benchmarks by using XcalableMP”, 2nd XcalableMP workshop, Oct. 2014 (in Japanese).
6. Miwako Tsuji and Mitsuhisa Sato, The extension of OmniRPC-MPI toward fault tolerant computation in a multi SMPD environment, 2014-HPC-146, Oct. 2014 (in Japanese).
7. Miwako Tsuji, XMP/YML for a multi SPMD programming environment, 2nd XcalableMP workshop, Oct. 2014 (in Japanese).
8. Masahiro Nakao, Hitoshi Murai, Hidetoshi Iwashita, Takenori Shimosaka, Akihiro Tabuchi, Taisuke Boku and Mitsuhisa Sato. SC14 The 2014 HPC Challenge Awards BoF, New Orleans, LA, USA, Nov., 2014.
9. Masahiro Nakao, “Evaluation of XcalableMP by using HPC Challenge Benchmarks”, PC cluster workshop in Osaka, Feb. 2015 (in Japanese).
10. Miwako Tsuji and Mitsuhisa Sato, An investigation of workflow scheduling to realize fault tolerant in a multi SPMD programming environment, 2015-HPC-148, Mar. 2015 (in Japanese)
11. Miwako Tsuji, Fault Tolerance features of YML-XMP, Workshop on Language and Programming Paradigm for Exascale Applications, Mar. 2015
12. Miwako Tsuji, Fault resilient in a multi SPMD programming environment FP2C, 2nd workshop on middleware for fault tolerant, Mar. 2015 (in Japanese)
13. Masahiro Nakao, Hitoshi Murai, Hidetoshi Iwashita, Takenori Shimosaka, Mitsuhisa Sato, “Evaluation and Implementation of HPC Challenge Benchmarks by using PGAS language XcalableMP, ” 2015-HPC-148(21), Mar. 2015, (in Japanese).
14. Masahiro Nakao, Hitoshi Murai, Miwako Tsuji, Takenori Shimosaka, Ryuhei Harada, Tetsuya Odajima, Akihiro Tabuchi, Keisuke Tsugane, Laurence Beaude, Mitsuru Ikei, Taisuke Boku, Mitsuhisa Sato. “Development and evaluation of parallel language for cluster system equipped with accelerators”. 6th cross-disciplinary symposium of computational science – development, assimilation, and construction of new knowledge, Oct. 2014 (in Japanese).
15. Miwako Tsuji and Mitsuhisa Sato, Programming model for post peta sacale computing, 6th cross-disciplinary symposium of computational science - development, assimilation, and construction of new knowledge, Oct. 2014 (in Japanese).
16. Hidetoshi Iwashita. Coarray Features Contained in Parallel Language XcalableMP. Short Lecture at the booth of SC2014, November, 2014.
17. Hitoshi Murai, Masahiro Nakao, Takehiro Shimosaka, Akihiro Tabuchi, Taisuke Boku, and Mitsuhisa Sato, “XcalableACC - a Directive-based Language Extension for Accelerated Parallel Computing,” SC14, New Orleans, LA, USA, Nov. 2014.

(5) Patents and Deliverables

- Omni XcalableMP compiler ver. 0.9.1 (registered as an AICS-supported software)

Processor Research Team

1. Team members

Makoto Taiji (Team Leader)
Yousuke Ohno (Senior Research Scientist)
Noriaki Okimoto (Senior Research Scientist)
Mitsugu Araki (Research Scientist)
Gentaro Morimoto (Research Scientist)
Takao Otsuka (Research Scientist)
Yoshinori Hirano (Research Scientist)
Tomoki Kobori (Postdoctoral Researcher)
Yohei Koyama (Postdoctoral Researcher)
Akiko Tamon (Research Associate)
Aki Hasegawa (Research Associate)
Kei Taneishi (Technical Staff)
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.

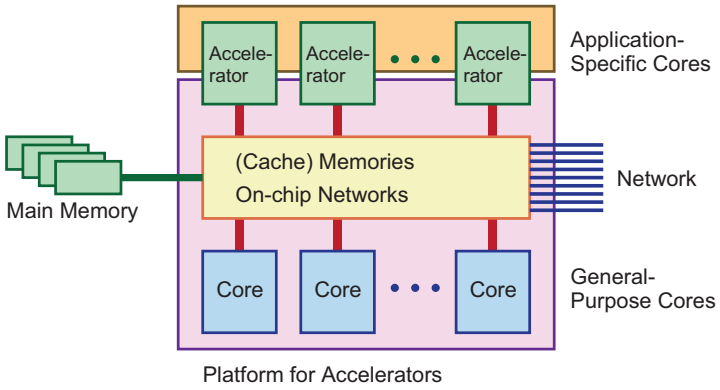


Fig. 1. Diagram of platform for accelerators.

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.

We have also performed the researches to improve rational drug discovery by high-performance computing. In addition, a research for large-scale machine learning of clinical data was also performed. These researches were done in collaboration with Prof. Yasushi Okuno (Kyoto University, senior visiting scientist of AICS).

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 full MDGRAPE-4 system. This year we have constructed the total system of the MDGRAPE-4 with 512 chips mounted on 64 boards. 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.

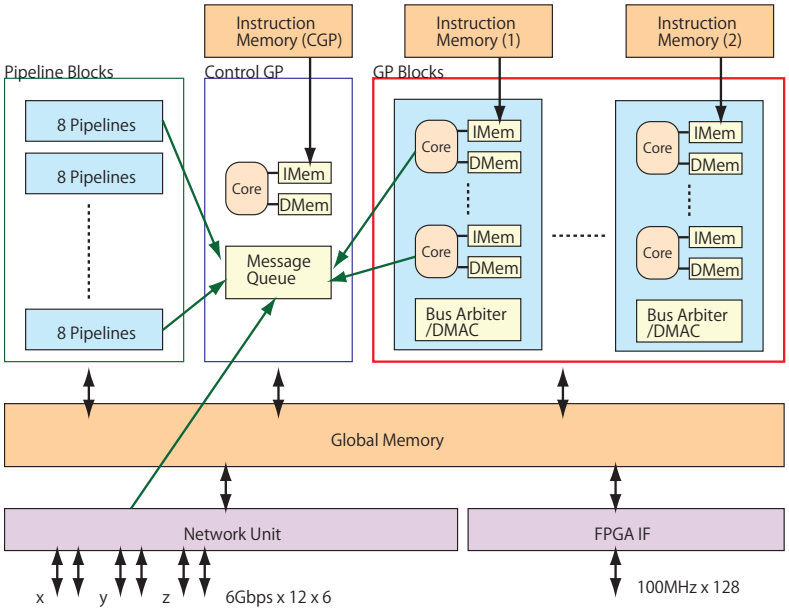


Fig. 2. Block diagram of MDGRAPE-4 SoC.

Fig. 3. MDGRAPE-4 system with 512 chips in 64 subracks.

3.2 Application Optimization on K computer

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

3.3 Accelerator for Deep Neural Networks

We have started to develop an accelerator for deep neural networks. We evaluated the Network-on-Chip based architecture and implemented it on the Field-Programmable Gate Array.

3.4 Drug discoveries using high-performance computing

We have validated the utility of molecular simulation of protein-drug binding using K computer. In chemotherapy of advanced fusion-type non-small-cell lung cancer, several drug resistance mutations have been found in the anaplastic lymphoma kinase (ALK) tyrosine kinase domain, but its molecular mechanisms remain unclear. Thus, we computationally modeled tertiary structures of drug-resistant ALK mutants, and evaluated binding affinities (ΔG) between the ALK mutants and anti-cancer drugs using MP-CAFEE (Massively Parallel Computation of Absolute binding Free Energy) method. Calculated ΔG correlated well with drug efficacy obtained from cell-based assay, suggesting that decreases in the binding affinity caused by amino acid mutations on ALK may be a dominant cause of the drug resistance. The molecular simulation using high-performance computing will be next applied to drug design for the drug-resistant mutants.

3.5 Clinical informatics using machine learning

Several studies have reported a lack of benefit in continuing cancer chemotherapy during a patient's pre-death terminal phase, and that late therapy might increase the risk of emergency hospital care. Therefore we attempted to establish a prognosis model to predict a patient's death that could help physicians make a decision to discontinue palliative chemotherapy by using longitudinal laboratory test data. We enrolled cancer patients who had received chemotherapy at the outpatient oncology unit of Kyoto University Hospital, and multivariate logistic regression analyses were executed to evaluate the efficiency of prognosis prediction and calculate a cutoff value that could suitably recommend discontinuation of treatment.

4. Schedule and Future Plan

In the next year, we will finish the MDGRAPE-4 Software 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 continue the drug design and medical application of high-performance computing with

Prof. Yasushi Okuno, senior visiting scientist.

5. Publication, Presentation and Deliverables

(1) Journal Papers

1. Katayama R., Friboulet L, Koike S, Lockerman EL, Khan TM, Gainor JF, Iafrate AJ, Takeuchi K, Taiji M, Okuno Y, Fujita N, Engelman JA, Shaw AT., “Two novel ALK mutations mediate acquired resistance to the next-generation ALK inhibitor alectinib”, Clinical Cancer Research, Vol.20. No.22, P.5686-5696 (2014)

(2) Conference Papers

(3) Invited Talks

2. 荒木望嗣、中津井雅彦、広川貴次、金井千里、佐藤美和、岡本敦之、服部一成、志水隆一、奥野恭史："新薬開発を加速する「京」インシリコ創薬基盤の構築”、国際ワークショップWINTech2015、神戸、 2015年3月12日.
3. 荒木望嗣、中津井雅彦、広川貴次、金井千里、佐藤美和、岡本敦之、服部一成、志水隆一、奥野恭史：”分子動力学シミュレーションの基礎と創薬分野での応用研究”、日本化学会情報化学部会主催　第二回若手の会、東京、2014 年 11 月 29 日.

(4) Posters and presentations

1. 荒木望嗣、中津井雅彦、広川貴次、金井千里、佐藤美和、岡本敦之、服部一成、志水隆一、奥野恭史：”新薬開発を加速する「京」インシリコ創薬基盤の構築”、HPCI 第 1 回成果報告会、東京、10/31(2015)

(5) Patents and Deliverables

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)
Daichi Mukunoki (Post Doctoral Researcher)
Daisuke Takahashi (Senior Visiting Researcher)
Franz Franchetti (Visiting Researcher)
Yoshio Okamoto (Visiting Researcher)
Yukiko Akinaga (Assistant)

2. Research Activities

The Large-scale Parallel Numerical Computing Technology Research Team conducts research and development of large-scale, highly parallel and high-performance numerical software for K computer. Simulation programs require various numerical techniques to solve systems of linear equations, to solve eigenvalue problems, to compute and solve non-linear equations, and to do fast Fourier transforms. In order to take advantage of the full potential of K computer, we must select pertinent algorithms and develop a software package by assembling numerical libraries based on the significant concepts of high parallelism, high performance, high precision, resiliency, and scalability. Our primary mission is to develop and deploy highly parallelized and scalable numerical software on K computer, namely KMATHLIB. It comprises several components such as for solving

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

The K-specific topics and technical matters for emerging supercomputer systems 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 a tight collaboration among computational science (simulation), computer science (hardware and software), and numerical mathematics. Our final goal is to establish fundamental techniques to develop numerical software libraries for next generation supercomputer systems based on strong cooperation within AICS.

3. Research Results and Achievements

Following published annual reports 2012-13 and 2013-14, we focus on the update and the latest results of running projects, 1) development of KMATHLIB, 2) development of EigenExa, 3) investigation of the FDTD related method, and 4) other fundamental studies for optimization of BLAS kernels by automatic parameter tuning. The plans and the publication list are also presented in the last section.

3.1. KMATHLIB Project

1) Development of KMATHLIB for the integration of OSS packages

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

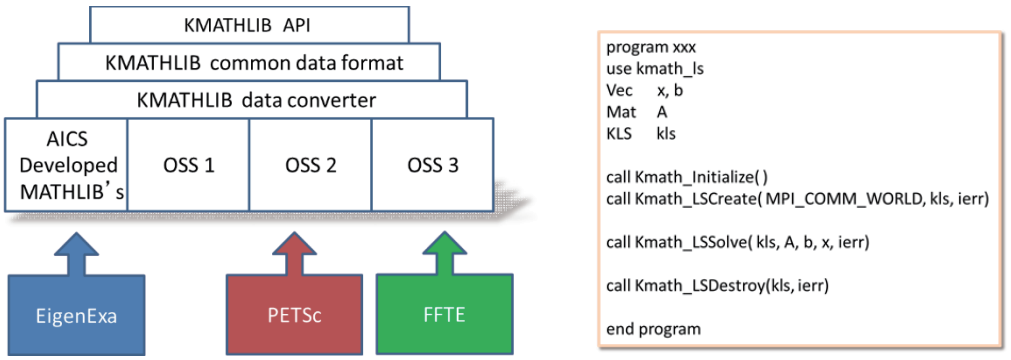


Figure 1. The structure of the KMATHLIB package (left) and a code example (right)

The left picture in Figure 1 depicts the schematic of KMATHLIB. KMATHLIB-API is on the top layer and is accessed by users directly. Since we designed a flexible plugin mechanism and API's, favorite OSS can be plugged in like the bottom highlighted part of Figure 1. KMATHLIB-API can conceal the differences of API's and data structures. The right part of Figure 1 shows an example of KMATHLIB-API. As Figure 1 (right) illustrates, KMATHLIB-API adopts a modern API style of

the standard numerical libraries, like PETSc and FFTW. Thus, we only have to use a unique procedure to use the numerical solver plugged in the KMATHLIB package. In this FY, we have updated the plugin mechanism, and it enables users to enhance the KMATHIB library according to their computational environment. Currently, the KMATHLIB library supports LAPACK, ScaLAPACK, EigenExa, PETSc, FFTW, FFTE, and SSL II as built-in libraries.

2) Enhancement of the KMATHLIB numerical libraries

Since FY2012-2013, we also have reviewed the parallel performance of the standard parallel OSS. We have concluded that most of OSS does not scale on a large number of processors (see the former annual reports in FY2012-2013 and FY2013-2014). Improvement of performance and enhancement of functionality is reported in this subsection.

As a part of the KMATHLIB project, we have carried out research on the development of a solver for generalized eigenvalue problems of banded matrices (GEPBs) $A\boldsymbol{x} = \lambda B\boldsymbol{x}$. In our solver, a new divide-and-conquer algorithm for GEPBs that is based on Elsner's idea is employed. The method has two advantages: i) its FLOPS count is smaller than the conventional method if the half bandwidth of the matrices is 3 or less, and ii) the most of the operations can be parallelized efficiently.

In FY2014-2015, we implemented the solver by OpenMP and evaluated the single node performance of our solver and conventional solvers (DSBGVD and DSYGVD in Intel MKL, as an optimized LAPACK implementation). Experiments are carried out on a standard workstation installed with two

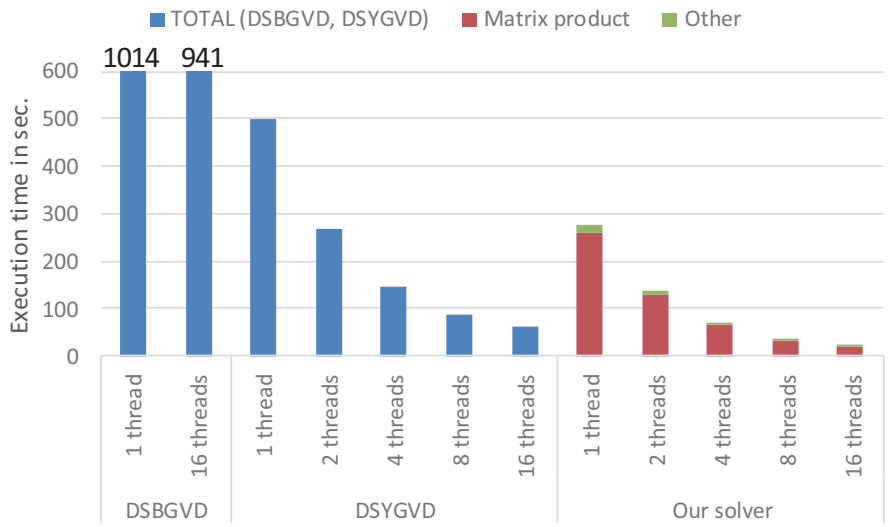


Figure 2. Comparison of the Execution time of solvers; DSBGVD and DSYGVD (from LAPACK), and our proposed solver.

Xeon E5-2660 CPUs (totally 16 cores). Figure 2 shows the execution time to compute all eigenpairs of a GEBP for pentadiagonal matrices (i.e. half bandwidth equals two). Our solver performs 3.2 times faster than the conventional solvers when using 16 threads. The speedup (defined by 'the execution time in the sequential mode' / 'the execution time in the thread-parallel mode') on our solver is higher than that of the conventional solvers. We also have developed a prototype implementation for Intel Xeon Phi and preliminary experiments have been done.

KMATH_RANDOM is a pseudo real random number generator for highly parallel computers such as K computer. KMATH_RANDOM is based on dSFMT, which is an open source code written by Prof. Saito and Prof. Matsumoto in Hiroshima University. KMATH_RANDOM manages random number generators running in each MPI process. On each MPI process, KMATH_RANDOM reads a file called 'jump file' and generates real random numbers independently. KMATH_RANDOM has been released on our team website since December 2014.

In FY2014, we studied the performance bottleneck of KMATH_RANDOM that we reported in last year. Figure 3 shows the execution time and the breakdown (initialization time and generation time of the random numbers) of each process to generate 1 billion random numbers in total with 1,000 MPI processes. Although the generation times are identical in appearance among processes, the initialization times in some nodes are much larger than the median time, and thus it causes the performance degradation of KMATH_RANDOM.

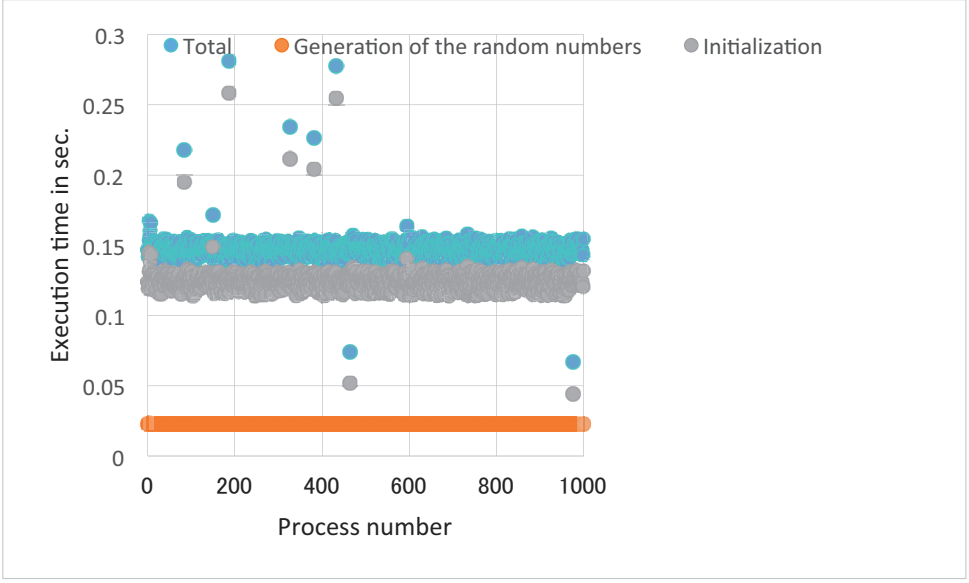


Figure 3. Execution time of each process and its breakdown.

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 have conducted mainly a part of the development of a high performance parallel dense eigenvalue solver, namely EigenExa. The EigenExa library was released in August 2013. In this FY 2014-2015, we mainly promoted the library and evaluated it on some supercomputer systems. Besides, we have investigated fundamental algorithms in numerical linear algebra such as the QR factorization (or orthonormalization).

1) Detailed performance evaluation of the EigenExa eigensolver

In this FY, we have evaluated the performance of our EigenExa eigensolver in detail, mainly with the focus on the difference between the *eigen_s* routine, which is based on the traditional tridiagonalization, and the *eigen_sx* routine, which employs a novel approach via pentadiagonalization. The latter has advantages in the step of transforming the input matrix into a penta/tridiagonal matrix. However, the latter requires more cost for computing the eigenvalues and eigenvectors of the pentadiagonal matrix by the divide-and-conquer method than the former. In order to clarify the potential of our new approach, it is important to evaluate the performance of both routines and to compare them in detail.

Figure 4 shows the breakdown of the execution time of eigen_s and eigen_sx on the Oakleaf-FX system (at The University of Tokyo). We used its 4,800 nodes and computed all eigenvalues and eigenvectors of a matrix with N=230,000. The graph clearly illustrates that two steps, namely tri/pentadiagonalization and divide-and-conquer steps, are dominant. It also indicates the advantages of eigen_sx (i.e. less flop and communication costs in the pentadiagonalization step) and the disadvantage (i.e. the additional cost in the divide-and-conquer step). By combining these detailed performance results and the expected specifications of post-petascale systems, we could predict the performance of these two routines on upcoming systems, which would strengthen the effectiveness of our new approach.

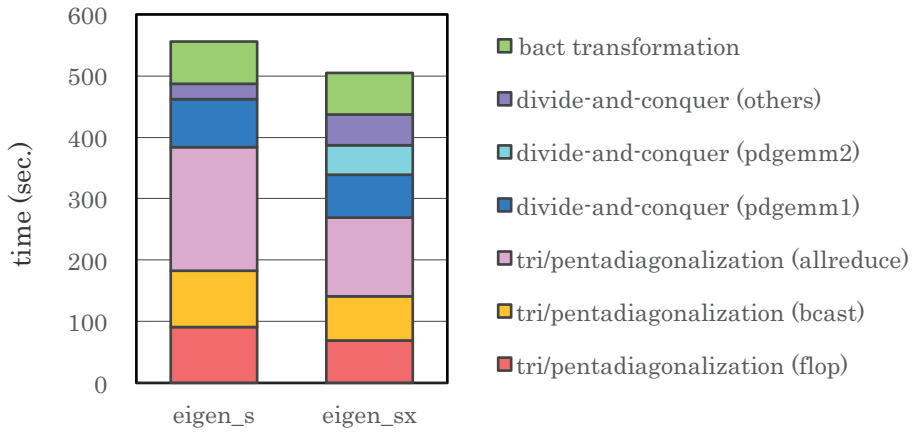


Figure 4. Breakdown of the execution time of eigen_s and eigen_sx. (N=230,000, and using 4,800 nodes of Oakleaf-FX)

2) Studies on the Cholesky QR factorization for tall-skinny QR factorizations

Computing the QR factorization of tall and skinny matrices (tall-skinny QR factorization) is required in blocked subspace projection methods for solving large and sparse eigenvalue problems. The Cholesky QR factorization is an algorithm that computes the QR factorization through the Cholesky factorization of the Gram matrix of the input matrix: $A^{\top}A \rightarrow R^{\top}R$. This algorithm consists almost entirely of Level-3 BLAS operations (e.g. matrix-matrix multiplication) and requires only one global reduction in parallel computation. These features mean that Cholesky QR is very suitable for recent large-scale parallel systems such as K computer. However, it is well-known that Cholesky QR has a serious numerical instability: the loss of orthogonality of the computed Q factor grows rapidly as the condition number of the input matrix increases. Therefore, it has been a consensus that Cholesky QR is fast but not practical.

In this FY, through collaboration with researchers in the field of applied mathematics, we have studied an algorithm that simply repeats the Cholesky QR algorithm twice, which we call the CholeskyQR2 algorithm. We have pointed out that CholeskyQR2 is as stable as conventional stable algorithms (e.g. the Householder QR factorization) until the condition number of the input matrix is less than about 10^8 (see Figure 5). In our evaluation on K computer, CholeskyQR2 is still faster than the TSQR algorithm (see Figure 6), which is a stable and communication-avoiding algorithm. These results totally indicate that CholeskyQR2 has a remarkable potential to be used in practical computations.

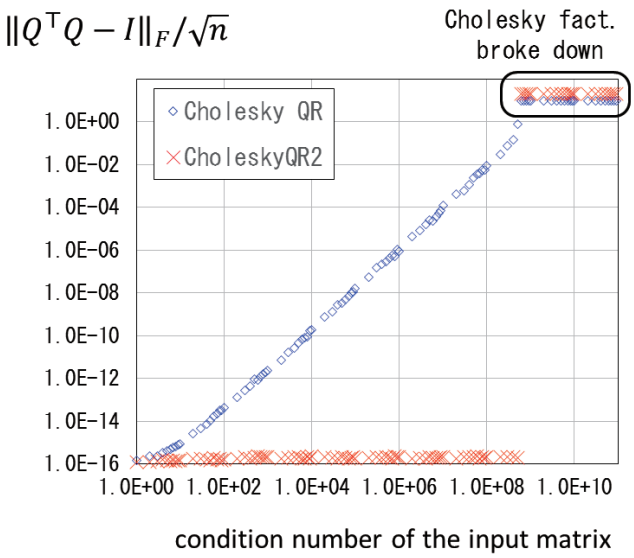


Figure 5. Numerical stability of CholeskyQR2.
(m=2,097,152, n=64, and #processes=8,192 on Oakleaf-FX system)

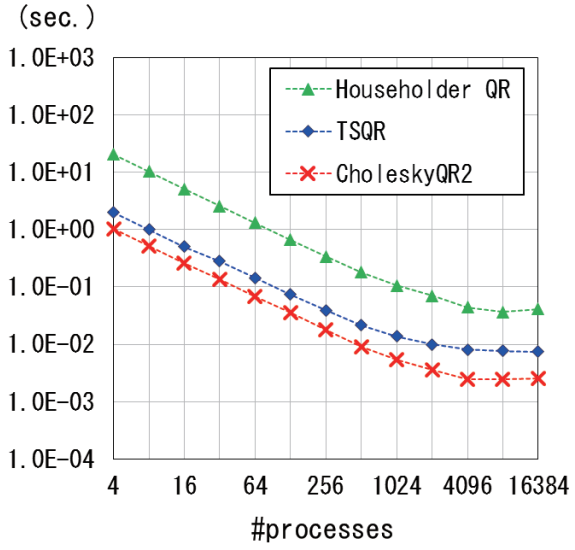


Figure 6. Parallel performance of CholeskyQR2 on the K computer.
(m=4,194,304, and n=64)

3.3 Investigation of the FDTD Related Methods

1) FDTDM (finite-difference time-domain method)

Recently, an electric power problem is one of the important issues for industrial and environmental engineering communities. A large-scale numerical simulation reveals various unknown factors. It is widely known that the finite-difference time-domain method (FDTDM) is applied for numerical simulations of electromagnetic wave propagation phenomena. Since most of the preexistent FDTDM software is commercial (not free software), it is quite hard to modify the simulation code to analyze

a phenomenon by new approaches. Thus, we recognized that it is one of the key issues to develop open source software based on FDTDM for K computer. In FY2014-2015, we surveyed papers in computational electromagnetics.

2) MTDM (meshless time-domain method)

In FDTDM, nodes of electric and magnetic fields are arranged based on an orthogonal mesh like a staggered mesh. Hence, it has restrictions in practice when we treat a complex shaped domain. On the other hand, the radial point interpolation method (RPIM), which is one of the meshless methods, can be theoretically applied to an arbitrarily shaped domain. The meshless time-domain method (MTDM) based on RPIM has useful features inherited from FDTMD and RPIM. However, we have open issues about the relation between two vital functions, the weight function and the shape function, which appear in MTDM. For example, the most suitable weight function to generate the shape function and appropriate arrangement of the nodes of electric and magnetic field must be clarified. In FY2014-2015, we have evaluated the transmission loss of electromagnetic wave propagation in a straight waveguide, numerically. In the simulation, we varied the weight function with a multi-quadratic, a reciprocal of the multi-quadratic, a quadratic spline, and an exponential function. As a result, we obtained that the quadratic spline function is the most suitable for MTDM. Also, we improved the acceleration method (we proposed originally in FY2013-2014) for the generation of shape functions. Two things are essential for the improvement, i) enlargement of the computational domain in which shape functions are reused, ii) the reduction of the number of times of shape function generations. The modified method performs excellently on a multicore processor, and we confirmed up to 100x speedup compared with the conventional method.

3.4 A study for development of multifunctional linear algebra libraries on future architectures

Traditional linear algebra libraries such as Basic Linear Algebra Subprograms (BLAS) and Linear Algebra PACKage (LAPACK) are still essential building blocks for computational science. However, nowadays they are required not only to achieve high performance with scalability, but also to support accurate, fault-tolerant, and energy-efficient computations toward the Exa-scale computing. We are conducting a study for the development of multifunctional linear algebra libraries dealing with these issues by utilizing some technologies such as auto-tuning and mixed precision calculation (including higher-precision compared to the hardware supported precision).

1) Implementation of fast GEMV routines with online auto-tuning on GPUs

We assume that auto-tuning is one of the most prominent technologies for the efficient

development of high performance multifunctional numerical libraries on complex architectures such as many-core processors. We proposed a sophisticated implementation of GEMV, a BLAS routine for computing dense matrix-vector multiplication, for NVIDIA GPUs. Some existing implementations have performance fluctuations depending on the input matrix size. On the other hand, our implementation achieved both higher throughput and better performance stability with respect to entry size of the matrix on multiple GPU architectures (Fermi, Kepler, and Maxwell architectures) by introducing an auto-tuning method that determines the optimal thread block size for the GEMV kernel. Our auto-tuning is "online" auto-tuning, which does not need trial executions to determine the tuning parameters by using a theoretical performance model. In the coming year, we will extend the experiences in this work on GPUs to other many/multi-core architectures such as Intel Xeon Phi and K computer.

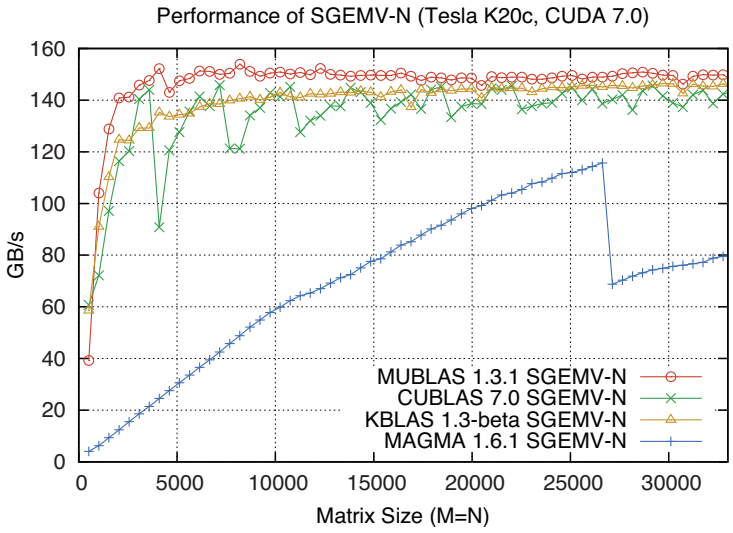


Figure 7. Performance comparison of SGEMV-N (single-precision GEMV for non-transposed matrix) on an NVIDIA Tesla K20c (Kepler architecture GPU). MUBLAS 1.3.1 (red-line) is our implementation.

2) Acceleration of DGEMM with software-emulated double-precision floating-point arithmetic on Maxwell architecture GPUs

In 1971, Dekker proposed double length floating-point arithmetic to compute a floating-point arithmetic with 2N length significand using a floating-point arithmetic with N length significand. The method is often used for accurate computation and is also known as double-double arithmetic by Bailey to compute quadruple-precision arithmetic using double-precision arithmetic. We used this method to accelerate DGEMM, a BLAS routine for computing double-precision dense matrix multiplication, on the NVIDIA Maxwell architecture GPU, the double-precision performance of which is 1/32 of single-precision. As a result, we showed that

the DGEMM with the software-emulated double-precision arithmetic outperforms the vendor implementation computed in hardware FPU on the GPU.

3) Development of parallel quadruple-precision BLAS

We are developing some quadruple-precision numerical libraries using double-double arithmetic for accurate computation on K computer. P-QPBLAS is the parallel version of QPBLAS, a quadruple-precision BLAS implementation using double-double arithmetic by Japan Atomic Energy Agency (JAEA). The prototype version of the P-QPBLAS has been implemented in the past year, and we are going to continue the development to release it in the future. However, there remain some issues in terms of the performance, and we recognize that some refactoring tools should be introduced to reduce the development cost.

4. Schedule and Future Plan

Our three main projects, KMATHLIB, EigenExa, and FDTD are still on-going works.

1) KMATHLIB project

To promote the KMATHLIB package, we recognize to support much useful plugged-in OSS. We plan to extend plugin solvers for, such as sparse linear equations, GEBPs, SVD for tensors. Urgent work related to this report is about GEBPs solver on distributed highly parallel computers such as the K computer, and we will soon release it as a part of KMATHLIB in FY2015-FY016. Furthermore, we also plan to release the solver for many core accelerators such as Intel Xeon Phi in FY2015 or later. Improvement of the performance of the generalized eigenvalue solver for dense matrix and random number generator, which are already released, must be our principal task in FY2015-2016.

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 continually. Furthermore, we recognize that it is also significant to improve the performance and scalability. Introducing the Communication Avoiding, Communication Hiding, and Synchronous Avoiding are prominent technologies. Also, a lightweight or flexible implementation is also an important issue.

3) FDTD related method

Our MUST topics for the FDTD related project are to support a precise 3D simulation by using MTDM. In fact, to simulate side-effects of an MRI device to a human body have a significant impact on life science and medical engineering. We need to promote the FDTD related works, especially MTDM, which has been originally studied in our project. It shall enhance the research field in AICS.

4) Other issues

As we described from the startup of this project team, “Fault tolerance” or “Resilience” is one of the

key words for the peta-scale computing. Since K computer is very stable and not often halt due to the system failure, technical review, and feasibility studies are proceeding on other systems than K computer. From the viewpoint of the numerical library, we will establish a new algorithmic fault detection mechanism and its framework.

5. Publication, Presentation, and Deliverables

(1) Journal Papers

1. Yasuhiro Idomura, Motoki Nakata, Susumu Yamada, Masahiko Machida, Toshiyuki Imamura, Tomohiko Watanabe, Masanori Nunami, Hikaru Inoue, Shigenobu Tsutsumi, Ikuo Miyoshi, and Naoyuki Shida, "Communication-overlap techniques for improved strong scaling of gyrokinetic Eulerian code beyond 100k cores on the K-computer", International Journal of High Performance Computing Applications, Vol. 28, No. 1, pp. 73-86, 2014
2. Takemasa Miyoshi, Keiichi Kondo, and Toshiyuki Imamura, "The 10,240-member ensemble Kalman filtering with an intermediate AGCM", Geophysical Research Letters, Vol. 41, July 28 2014
3. Teruo Tanaka, Ryo Otsuka, Akihiro Fujii, Takahiro Katagiri, and Toshiyuki Imamura, "Implementation of d-Spline-based incremental performance parameter estimation method with ppOpen-AT", Scientific Programming, Vol. 22, No. 4, pp. 299-307, 2014

(2) Conference Papers

(Reviewed)

1. Chongke Bi, Kenji Ono, Kwan-Liu Ma, Haiyuan Wu, and Toshiyuki Imamura, "A Study of Parallel Data Compression Using Proper Orthogonal Decomposition on the K Computer", Proc. Eurographics Symposium on Parallel Graphics and Visualization (EGPGV2014), Swansea, UK, June 9-10, 2014.
2. Takeshi Fukaya, Toshiyuki Imamura, and Yusaku Yamamoto, "Performance Analysis of the Householder-type Parallel Tall-Skinny QR Factorizations toward Automatic Algorithm Selection", Proc. the Ninth International Workshop on Automatic Performance Tuning (iWAPT2014), pp.1-8, Eugene, USA, July 1, 2014
3. Takeshi Fukaya, Yuji Nakatsukasa, Yuka Yanagisawa, and Yusaku Yamamoto, "CholeskyQR2: A Simple and Communication-Avoiding Algorithm for Computing a Tall-Skinny QR Factorization on a Large-Scale Parallel System", Proc. the 5th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems (ScalA), pp.31-38, New Orleans, USA, November 17, 2014
4. Daichi Mukunoki, Toshiyuki Imamura, and Daisuke Takahashi, "Fast Implementation of

General Matrix-Vector Multiplication (GEMV) on Kepler GPUs", Proc. the 23rd Euromicro International Conference on Parallel, Distributed and Network- based Processing (PDP 2015), pp. 642-650, Turku, Finland, March 4, 2015

(Non-reviewed)

1. Takahiro Katagir, Koichi Takayama, Takashi Yonemura, Hiroki Kumahora, Mitsuyoshi Igai, Junichi Kitagami, Yoshiyuki Eguchi, Takeshi Fukaya, Yusaku Yamamoto, Junichi Iwata, Kazuyuki Uchida, Satoshi Oshima, and Kengo Nakajima, "Application of the communication-avoiding algorithm CAQR to the orthogonalization process in RSDFT and its evaluation", IPSJ SIG Tech. Rep. [High Performance Computing], Vol.2014-HPC-144, No.3, pp.1-6, May 19, 2014 (in Japanese)
2. Takeshi Fukaya and Toshiyuki Imamura, "A study on auto-tuning for the structured QR factorization appearing in the TSQR algorithm", the 19th Annual Meeting of Japan Society for Computational Engineering and Science, Proc. JSCES, Vol.19, 2014 (in Japanese)
3. Toshiyuki Imamura, Yusuke Hirota, Takeshi Fukaya, Susumu Yamada, and Masahiko Machida, "Communication Avoiding (CA) and Communication Hiding (CH) in a dense-matrix eigenvalue problem", the 19th Annual Meeting of Japan Society for Computational Engineering and Science, Proc. JSCES, Vol.19, 2014 (in Japanese).
4. Yoshiharu Ohi, Taku Itoh and Soichiro Ikuno, "Speedup for generation of shape function in Meshless Time Domain Method", the 19th Annual Meeting of Japan Society for Computational Engineering and Science, Proc. JSCES, Vol.19, 2014 (in Japanese).
5. Toshiyuki Imamura, Daichi Mukunoki, Susumu Yamada, and Masahiko Machida, "Implementation and evaluation of CUDA-xSYMV", IPSJ SIG Tech. Rep. [High Performance Computing], Vol. 2014-HPC-146, No. 14, pp.1-12, September 25, 2014 (in Japanese)
6. Daichi Mukunoki, and Toshiyuki Imamura, "Implementation and Evaluation of DGEMM using Double-Float Arithmetic on Maxwell Architecture GPUs", IPSJ SIG Tech. Rep. [High Performance Computing], Vol. 2014-HPC-147, No. 26 pp. 1-6, December 2014 (in Japanese)
7. Toshiyuki Imamura, Daichi Mukunoki, Susumu Yamada, and Masahiko Machida, "Performance evaluation of the fastest GPU-based eigensalue solver by selecting CUDA-BLAS's", IPSJ SIG Tech. Rep. [High Performance Computing], Vol. 2015-HPC-148, No.4 pp.1-9, February 23, 2015 (in Japanese)

(3) Invited Talks

1. Toshiyuki Imamura, "The EigenExa Library – High Performance & Scalable Direct

Eigensolver for Large-Scale Computational Science", International Supercomputing Conference (ISC14), HPC in Asia session, June 26, 2014

2. Takeshi Fukaya, "The Cholesky QR factorization in high-performance computing", the 12th Computational Mathematics Conference, Dec. 28, 2014 (in Japanese)

(4) Technical reports, Posters and Presentations

(Technical Reports)

1. Takeshi Fukaya and Toshiyuki Imamura, "Performance evaluation of the EigenExa eigensolver by using the 4800 nodes of the FX10 system", Super Computing News, The University of Tokyo, Vol. 16, No. 3, pp. 20-27, May 2014 (in Japanese)
2. Takeshi Fukaya, "Performance evaluation of a communication-avoiding QR factorization by using the 4800 nodes of the FX10 system", Super Computing News, The University of Tokyo, Vol. 16, No. 4, pp. 11-20, July 2014 (in Japanese)

(Posters)

1. Yoshiharu Ohi, Taku Itoh, and Soichiro Ikuno, "Numerical Investigations of 3D Electromagnetic Wave Propagation Phenomena Using Meshless Time Domain Method", the 16th Biennial IEEE Conference on Electromagnetic Field Computation (CEFC2014), May 27, 2014.
2. Daichi Mukunoki, Toshiyuki Imamura, and Daisuke Takahashi, "Fast Implementation of SGEMV on Kepler Architecture GPUs", GTC Japan 2014, Tokyo, Japan, July 16, 2014 (in Japanese)
3. Takeshi Fukaya, "QR factorizations based on the Cholesky factorization", the 8th Kobe University Cooperative Division Symposium, Kobe Japan, September 11, 2014 (in Japanese)
4. Yusuke Hirota, "On Decomposition of Perturbation Matrices in Divide and Conquer Method for Generalized Eigenvalue Problems of Banded Matrices", the 8th Kobe University Cooperative Division Symposium, Kobe, Japan, September 11, 2014 (in Japanese)
5. Yoshiharu Ohi, and Soichiro Ikuno, "Numerical Investigation of Electromagnetic Wave Propagation Phenomena using 3D Meshless Time Domain Method", the 24th International Toki Conference (ITC-24), Toki, Japan, November 6, 2014
6. Takeshi Fukaya, "Modeling the performance of parallel dense eigensolvers on peta/post-petascale systems", JST/CREST International Symposium on Post Petascale System Software (ISP2S2), Kobe, Japan, December 2, 2014
7. Takeshi Fukaya, and Toshiyuki Imamura, "Performance evaluation of the EigenExa dense eigensolver on the K computer", the 5th AICS International Symposium, Kobe, Japan, December 8-9, 2014

8. Yusuke Hirota, and Toshiyuki Imamura, “Development of High Performance Parallel Real Random Number Generator KMATH_RANDOM”, the 5th AICS International Symposium, Kobe, Japan, December 8-9, 2014
9. Toshiyuki Imamura, Daichi Mukunoki, Narimasa Sasa, Susumu Yamada, and Masahiko Machida, “Pseudo-Quadruple precision extended mathematics Package, QP-Pack”, Annual Meeting on Advanced Computing System and Infrastructure (ACSI 2015), Tsukuba, Japan, January 26-28, 2015 (in Japanese)
10. Daichi Mukunoki, Toshiyuki Imamura, and Daisuke Takahashi, “Fast Implementation of SGEMV with Matrix Size Independent Performance on Kepler and Maxwell Architecture GPUs”, Annual Meeting on Advanced Computing System and Infrastructure (ACSI 2015), Tsukuba, Japan, January 26-28, 2015 (in Japanese)
11. Shin’ichi Sasaki, Akihiro Fujii, Teruo Tanaka, Daichi Mukunoki, and Toshiyuki Imamura, “Acceleration of Quadruple precision arithmetic on K supercomputer system”, Annual Meeting on Advanced Computing System and Infrastructure (ACSI 2015), Tsukuba, Japan, January 26-28, 2015 (in Japanese)
12. Yoshiharu Ohi, Yoshihisa Fujita, Taku Itoh, and Soichiro Ikuno, “Numerical Investigation of Influence of Node Alignment on Stable Calculation for Meshless Time Domain Method”, SIAM Conference on Computational Science and Engineering (CSE15), Salt Lake City, USA, March 14-18, 2015.
13. Daichi Mukunoki, ToshiyukiImamura, and DaisukeTakahashi, “High-Performance GEMV and SYMV with Auto-Tuning for Performance Stabilization on Multiple GPU Generations”, GPU Technology Conference (GTC 2015), San Jose, USA, March 17, 2015
14. Toshiyuki Imamura, “The EigenExa library: dense eigenvalue solver for post-petascale computing”, SSExa2015, Greifswald, Germany, March 22-25, 2015

(Oral presentations)

1. Takeshi Fukaya, “Communication-avoiding QR factorizations and related auto-tuning”, ATOS9, Tokyo, Japan, May 5, 2014 (in Japanese)
2. Toshiyuki Imamura, Yusuke Hirota, Takeshi Fukaya, Susumu Yamada, and Masahiko Machida, “EigenExa: high performance dense eigensolver, present and future”, the 8th International Workshop on Parallel Matrix Algorithms and Applications (PMAA2014), Lugano, Switerland, July 2-4, 2014
3. Yusuke Hirota and Toshiyuki Imamura, “Acceleration of Divide and Conquer Method for Generalized Eigenvalue Problems of Banded Matrices on Manycore Architectures”, the 8th International Workshop on Parallel Matrix Algorithms and Applications (PMAA2014), Lugano, Switzerland, July 2-4, 2014.

4. Takeshi Fukaya, Yusaku Yamamoto and Toshiyuki Imamura, "An study on blocking techniques of Householder transformations and related communication-avoiding", Summer united Workshop on Parallel, distributed and cooperative Processing (SWoPP2014), Niigata, Japan, July 28, 2014 (in Japanese)
5. Takeshi Fukaya, Yuji Nakatsukasa, Yuka Yanagisawa and Yusaku Yamamoto, "Performance evaluation of the Cholesky QR factorization with reorthogonalization on large-scale parallel systems", 2014 JSIAM Annual meeting, Tokyo, Japan, September 3, 2014 (in Japanese)
6. Yoshiharu Ohi and Soichiro Ikuno, "Analysis of node arrangement on computational accuracy and numerical stability using Meshless Time Domain Method", 2014 JSIAM Annual meeting, Tokyo, Japan, September 3, 2014. (in Japanese)
7. Yuka Yanagisawa, Yuji Nakatsukasa, Takeshi Fukaya, Yusaku Yamamoto, Shinichi Oishi and Kannan Ramaseshan, "Shifted Cholesky QR factorization", 2014 JSIAM Annual meeting, Tokyo Japan, September 4, 2014 (in Japanese)
8. Takuma Kawamura, Yasuhiro Idomura, Hiroko Miyamura, Hiroshi Takemiya, and Toshiyuki Imamura, "Remote visualization of large-scale simulation results on K-computer using particle-based volume rendering", Annual meeting on Atomic Energy Society of Japan, Kyoto, Japan, September 8, 2014 (in Japanese)
9. Yoshiharu Ohi, and Soichiro Ikuno, "Influence of Weight Function to Numerical Precision in 3D Meshless Time Domain Method", the 33rd JSST Annual Conference (JSST2014), Kita-kyushu, Japan, October 29, 2014.
10. Toshiyuki Imamura, Yusuke Hirota, Takeshi Fukaya, Susumu Yamada, and Masahiko Machida, "Post Peta-scale dense eigenvalue solver", JST/CEST International Symposium on Post Petascale System Software, Kobe, Japan, December 3-4, 2014
11. Yoshiharu Ohi and Soichiro Ikuno, "Stability analysis of Meshless Time-Domain Method using Arbitrary node arrangement", the 23th MAGDA conference (MAGDA2014), Takamatsu, Japan, December 4, 2014. (in Japanese)
12. Toshiyuki Imamura, "Review on large-scale dense eigenvalue computation", 18th Symposium on Setouchi-rim JSIAM Local Research Group, Kurashiki, Japan, December 6, 2014 (in Japanese)
13. Yoshiharu Ohi, Taku Itoh, and Soichiro Ikuno, "Evaluation of Node Arrangement Based on Finite Element in Meshless Time-Domain Method", Nonlinearity/Visualization-Section Meeting in Workshop on developments of new simulation methods for plasma-wall interaction 2014, Toki, Japan, January 26, 2015. (in Japanese)
14. Takeshi Fukaya and Toshiyuki Imamura, "Performance evaluation of the EigenExa eigensolver on the Oakleaf-FX supercomputing system", Annual Meeting on Advanced

Computing System and Infrastructure (ACSI 2015), Tsukuba, Japan, January 27, 2015 (in Japanese, reviewed)

15. Takeshi Fukaya, "CholeskyQR2: an algorithm of the Cholesky QR factorization with reorthogonalization", 2015 Conference on Advanced Topics and Auto Tuning in High-Performance and Scientific Computing (2015 ATAT in HPSC), Taipei, Taiwan, February 27-28, 2015
16. Toshiyuki Imamura, "Automatic-tuning for CUDA-BLAS kernels parameter by multi-stage d-Spline", 2015 Conference on Advanced Topics and Auto Tuning in High-Performance and Scientific Computing (2015 ATAT in HPSC), Taipei, Taiwan, February 27-28, 2015
17. Takeshi Fukaya and Toshiyuki Imamura, "Performance Evaluation of EigenExa Dense Eigensolver on the Oakleaf-Fx Supercomputer System", SIAM Conference on Computational Science and Engineering (CSE15), Salt Lake City, USA, March 14, 2015
18. Toshiyuki Imamura, Takeshi Fukaya, Yusuke Hirota, Susumu Yamada and Masahiko Machida, "Numerical Eigenvalue Engine towards Extreme-scale Computing Era", SIAM Conference on Computational Science and Engineering (CSE15), Salt Lake City, USA, March 18, 2015
19. Yusuke Hirota, "Present State of Eigenvalue Solvers and Prospects for Post Peta-scale Systems", Cyber HPC Symposium, Suita, Japan, March 20, 2015 (in Japanese)

(5) Patents and Deliverables

Currently, we have released five OSS from our site as follows.

1. EigenExa, http://www.aics.riken.jp/labs/lpnctrt/EigenExa_e.html
2. KMATH_EIGEN_GEV, http://www.aics.riken.jp/labs/lpnctrt/KMATH_EIGEN_GEV_e.html
3. KMATH_RANDOM, http://www.aics.riken.jp/labs/lpnctrt/KMATH_RANDOM_e.html
4. ASPEN.K2, http://www.aics.riken.jp/labs/lpnctrt/ASPENK2_e.html
5. MUBLAS-GEMV, http://www.aics.riken.jp/labs/lpnctrt/ASPENK2_e.html

HPC Usability Research Team

1. Team members

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Masatomo Hashimoto (Research Scientist)
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Petr Bryzgalov (Research Scientist)
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Judit Gimenez (Visiting Scientist, Barcelona Supercomputing Center)
Sameer Shende (Visiting Scientist, University of Oregon)
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

In FY2013, we developed a web-based user-interface for the computing portal framework developed in FY2012-FY2013. With the web interface, software developers can easily publish their applications installed in HPC systems, and users are able to launch the published applications. The web-interface is designed to be flexible in the sense that it can be accessed by not only web browsers run on PCs, but also modern smartphones. Thus, users can launch and monitor their jobs through their smartphones, anywhere, anytime.

In FY2014, we enhanced the computing portal framework with container (virtual execution environment) technologies. In the original computing portal framework, software developers are able to publish their applications installed in HPC systems, but the installation of the applications have to be performed in a conventional manner. That is, the software developers have to copy and install their binary executables by themselves. In addition, they may have to install additional software/libraries that are required by their own programs, but it is sometimes difficult and/or even impossible because the administrators of the HPC systems usually do not allow the software developers to install such the software/libraries arbitrary. Another approach of installing software is to copy and build the binary executables from their source code, but it is sometimes troublesome and messy.

To address the abovementioned problem of installing software in HPC systems, we utilize container

(virtual execution environment) technologies. A *container* is a kind of lightweight virtual execution environment that is isolated from its host environment and other containers. In other words, in a container, users are able to freely modify the environment of the container, that is, system administrators can let the users install any software they need without compromising security/safety of their systems, in theory.

More specifically, we utilized and integrated Docker (http://docker.io), a container system built on the Linux kernel, with our computing portal framework. In the computing portal framework extended with Docker, software developers are able to download a Docker container image that contains a basic execution environment of a HPC system, freely modify the image (i.e., install software/libraries) in order to prepare the execution environment required to run their applications, install their applications, and upload back the image to the computing portal framework. When publishing the applications, the software developers are able to specify the uploaded container images to be instantiated when the applications are launched as jobs. Moreover, the software developers are able to publish not only their applications, but also their container images so that other software developers can use the images.

From viewpoint of deploying the computing portal framework, there remain three problems. First problem is that the current implementation does not provide an accounting mechanism. That is, there is no way to know which application is executed by whom or who is to be charged for consumed computing resources. This will be even more complex when multiple applications (published by multiple software developers) and multiple users are involved. Second problem is that the container system of Docker cannot run on the computing nodes of the K computer (or FX10) because their Linux kernel version is too old to execute Docker properly (while its login nodes are new enough). The problem can be solved by upgrading the Linux kernel, but it is not easy because the Linux kernel running on the K computer is extensively modified in order to address problems caused in massively parallel computing environments. Third problem is the operation policy of the K computer. The primary purpose of the K computer is to perform scientific computation, thus its operation policy focuses on executing such the computation efficiently and reliably. Therefore, it is hard to directly integrate our computing portal framework with the K computer. Instead, we are currently using FX10 of AICS Research Division for experiments.

In FY2015, we will continue to develop our computing portal framework. Especially, we plan to implement some kind of accounting mechanisms to our framework. We also plan to upgrade the Linux kernel of the computing nodes (of our FX10 and/or the K computer), but we recognize that it is extremely difficult.

3.2. Virtualization Techniques

1. Lightweight virtualization for testing/debugging parallel programs

Writing a program which makes full use of massively parallel HPC environments (e.g., the K computer) is extremely difficult because debugging parallel programs is a hard task due to inherent non-determinacy of parallel programs and hard-to-reproduce bugs. Moreover, writing massively parallel programs also tend to suffer from a performance problem. For example, even if a program scales well on a PC cluster system whose size is small-to-moderate, the program may not scale on massively parallel HPC systems. Even worse, the performance may severely degrade and will be worse than on a small PC cluster system or even a single PC. Actually, this is not uncommon and the reason is that communication costs between computing nodes may largely vary and sometimes incurs unacceptable heavy overheads.

In order to address the abovementioned 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.

There are two key ideas in our system: library-hooking and decentralized management of routing information. Library-hooking is a kind of virtualization technology which intercepts function calls for system operations, and modify their parameters and/or return values in order to trick the programs as if they run on in isolated multiple computing nodes, even though they run on a single physical computing node. More specifically, in our lightweight virtualization system, we mainly hook network related operations (and some file I/O) from user programs. 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 and requires no interaction with OS.

When implementing a lightweight network virtualization system, decentralized management of routing information is necessary in order to avoid maintaining routing information in a single or a few physical nodes. Our lightweight virtualization system has to manage routing information by itself because it virtualizes network environments. If the routing information is managed in a single physical node, all the other physical nodes have to ask the single node in order to correctly route network packets from one virtual node to another. Therefore, when the numbers of virtual nodes and physical nodes are huge, the single node will become a performance bottleneck and severely degrade the overall performance of our lightweight virtualization system.

More specifically, our lightweight virtualization system statically distributes the information which virtual node runs on which physical node before executing user programs on virtual computing nodes. In ordinary HPC systems, it is uncommon that computing nodes are directly allocated during job execution. In addition, in order to virtualize port numbers, our lightweight virtualization system let physical nodes exchange the information about virtualized port numbers when one virtual node on one physical node communicates with another virtual node on another physical node. In our

previous implementation of FY2013, we also distributed the information of the virtual port numbers statically before executing user programs by dividing the range of the available physical ports into disjoint ranges and allocating the divided range to each physical node. However, we recognized that this approach does not scale when the number of the physical nodes become huge. Thus, we applied the dynamic exchange approach as described above.

Based on the abovementioned approaches, in FY2014, we have implemented a prototype of our lightweight virtualization system. It successfully runs on conventional PC clusters and Fujitsu's FX10. On the K computer, it successfully runs 20000 virtual computing nodes on 1000 physical computing nodes. In theory, it must be able to run more virtual computing nodes on a single physical computing node and run on more physical computing nodes, but this is not possible so far because currently the K computer restricts the number of user processes on a physical computing node and the operating system kernel of the computing nodes of the K computer has a serious fault which is related to memory management.

In FY2015, we will continue the development of our system and evaluate it with more large numbers of virtual computing nodes and physical computing nodes. In addition, we 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. Container technologies for HPC

As slightly described in Sec. 3.1, container technologies are a kind of lightweight virtualization technology. Although they tend to be less efficient than the library-hooking approach described in the previous section (Sec. 3.2.1), they provide more complete image of virtual execution environments. For example, Docker (http://docker.io) provides multiple isolated virtual Linux execution environments on a host Linux system. Because Docker is built and depends on several functionalities provided by the Linux kernel, it is not able to host non-Linux virtual execution environments unlike full-virtualization technologies (e.g., KVM, QEMU, and so on), but far more efficient than them.

One big problem of the current typical HPC systems compared to today's so-called cloud services from viewpoint of software developers/publishers is that the HPC systems are less flexible and/or responsive. For example, they are not allowed to install and/or modify system/middleware programs in the HPC systems, while the cloud services provide fully-virtualized environments to them and they can freely modify the environments. In addition, the typical HPC systems are operated with conventional batch schedulers and it sometimes takes time to launch jobs, while the cloud services launch virtual execution environments instantly when requested by them.

The reason why the conventional HPC systems are less flexible and/or responsive is that their primary purpose is to compute scientific applications efficiently as much as possible, thus the

overheads that may be introduced by utilizing full virtualization technologies are unacceptable.
On the other hand, as described above, the recent advance in the container technologies achieves very small overheads yet provides sufficiently flexible virtual execution environments, thus we predict that the container technologies will play important role in forthcoming HPC usage.
Based on the abovementioned perspective, we are studying the possibilities of applying the container technologies (especially, Docker) to the HPC systems. More specifically, in FY2014, we continued to develop dockerIaaSTools (https://github.com/pyotr777/dockerIaaSTools), which enables us to easily setup isolated multiple virtual execution environments to which users are able to login via SSH. In addition, as an application of dockerIaaSTools, we extended K-scope (http://www.kcomputer.jp/ungi/soft/kscope/), which is a Fortran source code analysis tool developed by Software Development team of AICS, so that users are able to use the backend of K-scope that is installed in the remote server seamlessly as if it is installed in their local computers. Moreover, we also studying the internals of Docker and developed extensions that enable us to conserve storage space for storing/managing imaged of Docker containers (e.g., https://github.com/pyotr777/docker-registry-driver-git). Furthermore, as described above (in Sec. 3.1), we integrated Docker with our computing portal framework.
In FY2015, we will continue to study the possibility of applying the container technologies to the HPC systems. For example, we plan to study the possibility of running Docker on the computing nodes of the K computer (or FX10 of AICS Research Division), though it is difficult because the Linux kernel running on the computing nodes are too old to run Docker. We have to know (and decide) which is more practical, modify the Linux kernel of the K computer, or target the forthcoming next-generation super computer.

3.3. Program verification and analysis

1. Memory Consistency Model-Aware Program Verification

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

number of the threads/nodes that share a single address memory space.

From the viewpoint of program verification, there are two problems in handling relaxed memory consistency models. First problem is that the conventional program verification does not consider relaxed memory consistency models. Thus, they cannot be applied directly 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. Thus, it is very tedious to define and implement program verification for each CPU and programming languages of relaxed memory consistency models.

To address these problems, we have been studying 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. Then, we define various memory consistency models as additional axioms on the base model. In fact, 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.

Second approach is to design and implement a model checker that supports various relaxed memory consistency models based on the formal model of the abovementioned 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 examples programs of the specification manuals of the memory consistency models of 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, and 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.

In FY2014, we optimized the implementation of our model checker (McSPIN) so that it can be applied to larger programs than the original implementation. More specifically, we introduced 4 optimization approaches: enhancing guard conditions, disabling speculation when unnecessary, prefetching instructions if possible, and removing the global time counter. In addition, in FY2014, we also enhanced our Hoare-style logic with a conventional rely-guarantee style rule in order to make the logic more compositional. More specifically, we added a new rely-guarantee style parallel composition rule because the original parallel composition rule is not compositional, that is, it requires us to infer all possible interleavings of parallel processes.

2. Evidence-Based Performance Tuning

To get the maximum of HPC systems, it is inevitable to optimize the performance of applications. However, performance tuning for massively parallel HPC systems is very difficult because it is not apparent how to improve programs except for highly skilled programmers. In addition, generally speaking, modifying correctly working programs is a bothering task from the viewpoint of developers. Thus, performance tuning requires experienced craftsmanship, and relies on intuition and experience.

In order to address the problem, we have been working on *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 FY2014, we developed a code mining mechanism which finds optimization patterns from source code modification history. More specifically, it calculates differences before and after modification at the level of abstract syntax trees and stores them to database. Then, we are able to search optimization patterns by searching database by queries that represent the patterns. More concretely, we defined about 40 queries that include loop unrolling, loop fusion, loop fission, loop interchange, array merging, array dimension interchange, code hoisting, and so on. In addition we also created a so-called *tuning catalog*, which enumerates very small example programs that represents various optimization patterns for reference data. With the tuning catalog and several real tuning histories, we conducted a supervised learning (which is one of machine learning approaches) in order to suggest appropriate optimization approaches for a given source code and performance profiling data. More specifically, we solved a multi-label classification problem by translating it to multiple single-label classification problems with the binary relevance method and solving them with the k-NN algorithm. As feature vectors, we used the values of performance profiling data (e.g., cache-miss rate) and source code metrics (e.g., max loop depth). With an experiment with 469 tuning cases, we obtained satisfactory results, but the experiment was still too small to determine effectiveness of our approach.

In FY2015, we plan to conduct the more realistic experiment with larger number of applications by designing and implementing automatic collector of source code modification histories and their corresponding performance tuning data.

4. Schedule and Future Plan

In FY 2015, we will continue to improve the implementation of our computing portal. As described in Sec. 3.1, one problem of the current implementation is that it does not provide an accounting mechanism to know which application is executed by whom or who is to be charged for consumed computing resources. In order to address the problem, we plan to implement some kind of accounting mechanisms to our framework.

Regarding the virtualization technologies, we will continue to implement and evaluate the lightweight network virtualization framework for testing/debugging parallel programs. More specifically, we will evaluate our implementation on larger number of the physical computing nodes with larger number of the virtual computing nodes, on the K computer. In addition, we will also continue to design and implement a mechanism which tricks performance profiling tools so that they feel as if they run on physical computing nodes and emit profiling data which represents characteristics under the real parallel computing environments. As for the container technologies, we will continue to study the possibility of applying the container technologies to the HPC systems. In addition, we plan to pursue the possibility of upgrading the Linux kernel which runs on the computing nodes of our FX10 in order to fully leverage the power of the container technology (Docker).

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, and improve them. Regarding the evidence-based performance tuning, we plan to conduct a relatively larger-scale experiment with larger number of applications with more realistic source code modification histories to determine effectiveness of our approach. In addition, we also plan to design and implement automatic collector of source code modification histories and their corresponding performance tuning data.

In addition to the above mentioned individual research topics, we also plan to design/implement integration of the research results of the virtualization technologies and the software verification with the computing portal.

5. Publication, Presentation and Deliverables

(1) Conference Papers (Refereed)

1. 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), pp. 332-341, 2014.

2. Terai, M., Bryzgalov, P., Maeda, T., and Minami, K., "Extending Kscope Fortran Source Code Analyzer with Visualization of Peformance Profiling Data and Remote Parsing of Source Code", In Proceedings of the 6th International Symposium on Advances of High Performance Computing and Networking (AHPCN) within Inrternational Conference on High Performance Computing and Communications (HPCC-2014), pp. 878-885, 2014.
3. Abe, T. and Maeda, T., "Optimization of a General Model Checking Framework for Various Memory Consistency Models", In Proceedings of the 8th International Conference on Partitioned Global Address Space Programming Models (PGAS 2014), pp. 14:1 - 14:10, 2014.
4. Hashimoto, M., Mori, A., and Izumida, T., "A Comprehensive and Scalable Method for Analyzing Fine-grained Source Code Change Patterns", In Proceedings of the International Conference on Software Analysis, Evolution, and Reengineering (SANER 2015), pp. 351 - 360, 2015.
5. Hashimoto, M., Terai, M., Maeda, T., and Minami, K., "Extracting Facts from Performance Tuning History of Scientific Applications for Predicting Effective Optimization Patterns", In Proceedings of the 12th Working Conference on Mining Software Repositories (MSR 2015), To appear.

(2) Invited Talks

6. Hashimoto, M., "Towards Evidence-based Performance Tuning Assist", The 6th Symposium on Automatic Tuning Technology and its Application (ATTA 2014), 2014. (In Japanese)

(3) Presentations

7. Abe, T., "Program Verification for Formalized Relaxed Memory Consistency Models", The 31st Symbolic Logic and Computer Science (SLACS), 2014. (In Japanese)
8. Abet, T., "Towards Semi-automatic Theorem Proving Considering Memory Consistency Models", The 25th Algebra, Logic, Geometry and Informatics (ALGI), 2014. (In Japanese)
9. Hashimoto, M., "Constructing Finge-Grained Tuning Cases Database and Its Application for Prediction of Effective Program Optimizations", The 10th Autotuning Research Group's Open Academic Session (ATOS10), 2014. (In Japanese)
10. Kitayama, I., "Parallel File I/O Optimization with SIONlib", Japan Lustre Users Group 2014 (JLUG 2014), 2014.
11. Abe, T., "Compositional Parallel Program Logic for Relaxed Memory Consistency Models",

Workshop on Computer Science and Category Theory (CSCAT 2015), 2015.

(4) Deliverables

12. Boost library (http://www.boost.org/) ported to the K computer. Available on the K computer.
13. MapReduce-MPI library (http://mapreduce.sandia.gov) ported to the K computer. Available on the K computer.
14. MPI4Py library (http://mpi4py.scipy.org/) ported to the K computer. Available on the K computer.
15. NumPy library (http://www.numpy.org/) ported to the K computer. Available on the K computer.
16. Python (https://www.python.org/) ported to the K computer. Available on the K computer.
17. A Python wrapper library for EigenExa (http://www.aics.riken.jp/labs/lpnctrt/EigenExa_e.html) (updated). Available on the K computer.

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 potential μ in a quantitative way is an important task of lattice QCD. We are currently working on tracing the critical line in the parameter space of temperature, chemical potential and quark mass in 3 flavor QCD using the O(a) improved Wilson quark action and the Iwasaki gauge action. As a first step we have determined the critical end point at zero chemical potential μ=0. Our strategy is to identify at which temperature the Kurtosis of physical observable measured at the transition point on several different spatial volumes intersects. This method is based on the property of opposite spatial volume dependences of the Kurtosis at the transition point between the first order phase transition side and the crossover one. We have obtained T_E=133(2)(1)(3) MeV and $m_{PS,E}$=306(7)(14)(7) MeV for the temperature and the pseudoscalar meson mass at the critical end point. This is the world's first determination of the critical end point in 3 flavor QCD and a significant step forward in our understanding of the phase diagram. As a next step we have investigated the phase structure in the presence of finite chemical potential $\mu \neq 0$. We first focus on extracting the curvature of the critical line on the μ/T-$(m_{PS})^2$ plane. The strategy to determine the critical end point at fixed finite μ is the same as the μ=0 case. Note that we incorporate the phase contribution coming from the quark determinant with $\mu \neq 0$ by the reweighting method. We evaluate the phase of the determinant exactly by developing an efficient numerical method with the use of a dimensional reduction technique in the temporal direction. We also employ the multi-parameter reweighting method to trace the critical line in a wide range of the chemical potential. Figure 1 shows the behavior of the critical line in the μ/T-$(m_{PS})^2$ plane. Red and blue symbols denote two choices of the physical input to determine the lattice cutoff so that their difference represents a systematic uncertainty in the scale determination. We clearly observe the curvature of the critical line. Its value is extracted from the following fit form:

$$\left(\frac{m_{\mathrm{PS,E}}(\mu)}{m_{\mathrm{PS,E}}(0)}\right)^2 = 1 + \alpha_1 \left(\frac{\mu}{\pi T_{\mathrm{E}}(0)}\right)^2 + \alpha_2 \left(\frac{\mu}{\pi T_{\mathrm{E}}(0)}\right)^4$$

We obtain α_1=1.924(60) and α_1=2.148(39) for red and blue symbols, respectively.

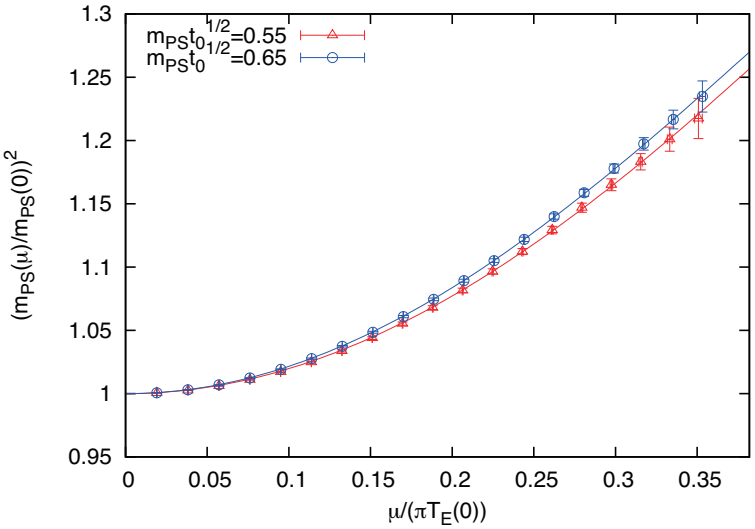


Figure 1: Critical line in the μ /T-$(m_{PS})^2$ plane. Red and blue symbols denote two choices of the scale setting.

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 in the world. 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, namely in experiment, 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 may disappear at some quark mass toward the physical value. We have investigated the quark mass dependence performing a simulation at m_π=0.30 GeV. Figure 2 show the $(m_\pi)^2$ dependence of the binding energies for ^{4}He nucleus (top left), ^{3}He nucleus (top right), deuteron (bottom left) and dineutron (bottom right) channels. Green star in each panel denotes the experimental value. We find that the ground states in all channels are bound states. Their binding energies show rather weak quark mass dependence in the

region from m_π=0.30 GeV to 0.51 GeV. The difference we observe from experiment may arise from various sources, either physical or computational in origin. A possible physical one is the heavier quark mass than experiment. Our results yield smaller binding energy in the dineutron channel than the deuteron channel in both cases of m_π=0.30 GeV to 0.51 GeV so that the former bound state may become unbound for further decrease of m_π. On the computational side, finite lattice spacing effects could be rather subtle. The repulsive property between the nucleons in the short distance, which is known to be important for the nucleus structure, could be strongly affected by such effects.

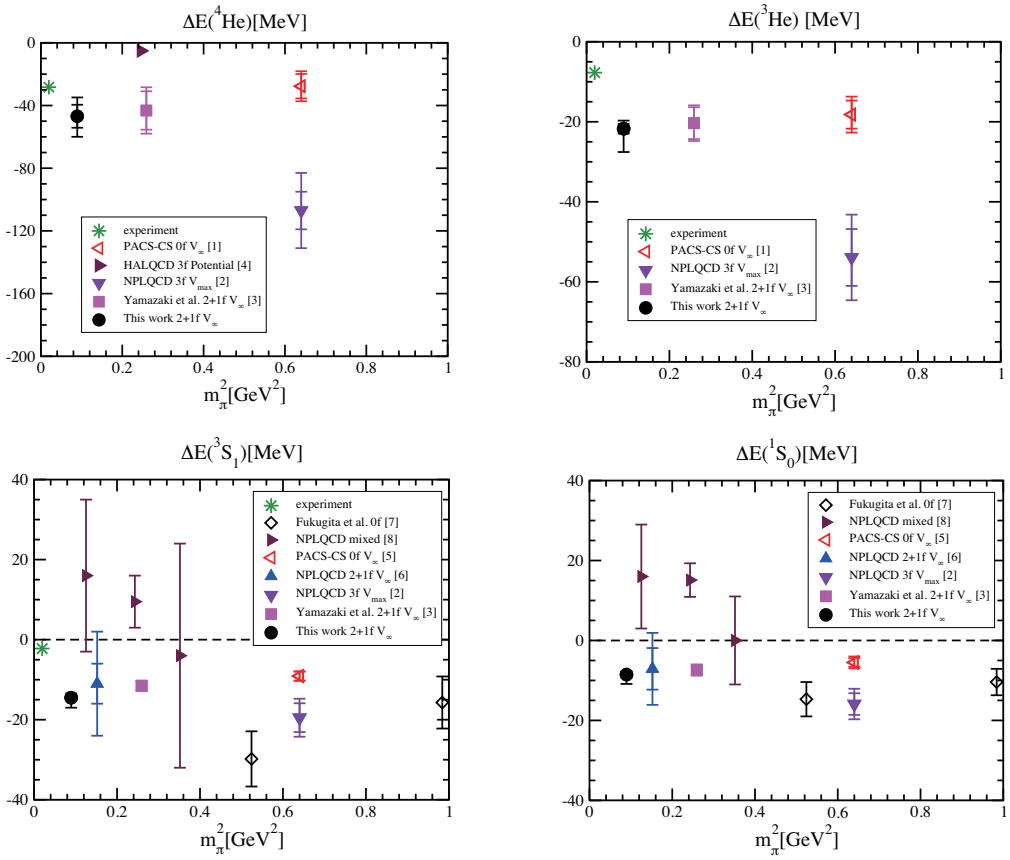


Figure 2: Binding energies for ^{4}He nucleus (top left), ^{3}He nucleus (top right), deuteron (bottom left) and dineutron (bottom right) channels as a function of $(m_\pi)^2$. Green star denotes the experimental value in each channel.

3.3. Development of algorithms and computational techniques

3.3.1. Application of z-Pares to lattice QCD on K computer

Eigenvalue problem for given large sparse matrix is common across various computational sciences including lattice QCD. Sakurai group in University of Tsukuba, who has been working on the eigenvalue problem for sparse matrices for a long time, is now developing a software package for massively parallel eigenvalue computation for sparse matrices called z-Pares (short for Complex

Moment-based Parallel Eigen-Solvers). From this fiscal year we started to apply z-Pares to a large scale calculation of lattice QCD on K computer. We have to solve the Wilson-Dirac equation Ax=b in lattice QCD, where A is an N×N complex sparse non-Hermitian matrix with N the number of four dimensional space-time sites multiplied by 12. In current typical simulations the dimension N is $O(10^9)$. z-Pares implements a complex moment based contour integral eigensolver. It computes eigenvalues inside a user-specified contour path on the complex plane and corresponding eigenvectors. In most cases of lattice QCD calculations our interest is restricted to O(10) eigenvalues around the origin so that lattice QCD should be a good example of application of z-Pares. Figure 3 shows a test result using a $12^3 \times 24$ lattice. Red circles denote the discretized contour consisting of 32 points on a circle with the radius of 0.01. We can obtain the eigenvalues and corresponding eigenvectors inside the contour. In Fig. 3 we find 8 eigenvalues denoted by black plus symbol. At present we work on tuning of algorithmic parameters in z-Pares using small or medium sizes of lattices. In next fiscal year, we plan to apply z-Pares to a 96^4 lattice used for a state-of-the-art calculation in lattice QCD.

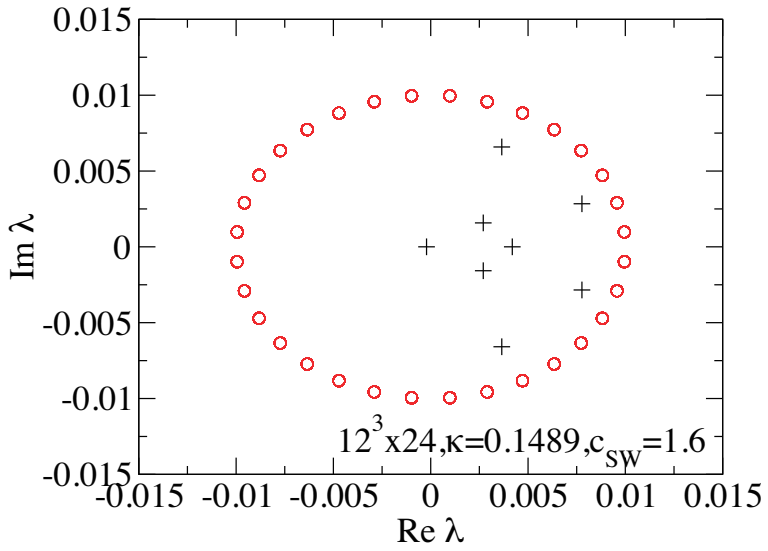


Figure 3: Eigenvalues of a Wilson-Dirac matrix with the lattice size of $12^3 \times 24$ around the origin in the complex plane. κ and c_{SW} denote the parameters to control the properties of the Wilson-Dirac matrix. Red circles denote the discretized contour on a circle with the radius of 0.01. Black plus symbol denotes the eigenvalues obtained by z-Pares.

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

The Monte Carlo simulation of lattice gauge theory is quite powerful to study nonperturbative phenomena of particle physics. However, when the action has an imaginary part like the θ term, it suffers from the numerical sign problem, failure of usual importance sampling techniques. The effect of the θ term on non-Abelian gauge theory, especially quantum chromodynamics (QCD) is

important, because it is related to a famous unsolved problem, “strong CP problem”. The difficulty is also shared with finite density lattice QCD. So development of effective techniques to solve or by-pass the sign problem leads to a lot of progress in the study of the QCD phase diagram at finite temperature and density. It is well-known that the θ term has a non-trivial contribution to Abelian gauge theory in two dimensions, too. Coleman argued that the (massive) Schwinger model, 2D QED, undergoes a phase transition at $\theta = \pi$ as m=g increases where m is the fermion mass and g is the coupling constant. Figure 4 illustrates the expected phase diagram of the Schwinger model with the θ term. Recently we successfully applied the Grassmann tensor renormalization group (GTRG) to the analysis on the one-flavor lattice Schwinger model in the Euclidean formulation. The GTRG method directly treats the Grassmann numbers without relying on the pseudofermion technique employed in the conventional hybrid Monte Carlo algorithm so that the computational cost is comparable to the bosonic case. Another virtue is that it does not suffer from the sign problem caused by the fermion determinant. We have extended the GTRG method to the case including the θ term, where the action becomes complex, and have succeeded in reproducing the expected phase structure at $\theta = \pi$ depicted in Fig. 4: When the fermion mass is large, there exists a first order phase transition and it terminates at m_c which has a second order phase transition belonging to the Ising universality class. It is shown that the GTRG is applicable to the physical system whose action is a complex number.

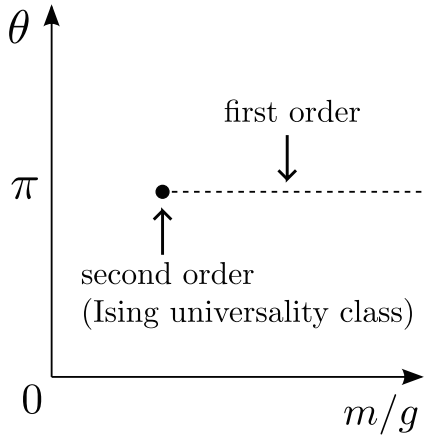


Figure 4: Expected phase diagram of Schwinger model with the θ term. The dotted line denotes a first order phase transition, which terminates at a second order phase transition point belonging to the Ising universality class.

4. Schedule and Future Plan

4.1. QCD at finite temperature and finite density

We are now investigating the critical surface in the parameter space of temperature, chemical potential and quark masses in 3flavor QCD. After that, we plan to explore the study of the phase

structure in 2+1 flavor QCD with the finite size scaling analysis.

4.2. Nuclei in lattice QCD

Our results at m_π=0.30 GeV in 2+1 flavor QCD show that the dineutron channel seems still bound. We currently make a large scale simulation at or around the physical quark mass. We also plan to investigate the possible systematic errors due to the finite lattice spacing.

4.3. Development of algorithms and computational techniques

4.3.1. Application of z-Pares to lattice QCD on K computer

In collaboration with Sakurai group at University of Tsukuba we plan to apply z-Pares to a 96^4 lattice used for a state-of-the-art calculation in lattice QCD.

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

We have demonstrated that the GTRG method is efficient even for the complex action employing the Schwinger model with the θ term. Next step is an extension to various spin models and non-Abelian lattice gauge theories on higher dimensions.

5. Publication, Presentation and Deliverables

(1) Journal Papers

1. X.-Y. Jin, Y. Kuramashi, Y. Nakamura, S. Takeda, and A. Ukawa, "Critical endpoint of the finite temperature phase transition for three flavor QCD", Physical Review D91 (2015) 014508.
2. X.-Y. Jin, Y. Kuramashi, Y. Nakamura, S. Takeda, and A. Ukawa, " Curvature of the critical line on the plane of quark chemical potential and pseudo scalar meson mass for three-flavor QCD", arXiv:1503.00113 [hep-lat].
3. R. Horsley, Y. Nakamura, A. Nobile, P.E.L. Rakow, G. Schierholz, and J.M. Zanotti, "Nucleon axial charge and pion decay constant from two-flavor lattice QCD", Physics Letters B732 (2014) 41.
4. P.E. Shanahan, A.W. Thomas, R.D. Young, J.M. Zanotti, R. Horsley, Y. Nakamura, D. Pleiter, P.E.L. Rakow, G. Schierholz, and H. Stüben, "Magnetic form factors of the octet baryons from lattice QCD and chiral extrapolation", Physical Review D89 (2014) 074511.
5. A. J. Chambers, R. Horsley, Y. Nakamura, H. Perlt, D. Pleiter, P. E. L. Rakow, G. Schierholz, A. Schiller, H. Stüben, R. D. Young, and J. M. Zanotti, "Feynman-Hellmann approach to the spin structure of hadrons", Physical Review D90 (2014) 014510.
6. A.J. Chambers, R. Horsley, Y. Nakamura, H. Perlt, P.E.L. Rakow, G. Schierholz, A. Schiller, and J.M. Zanotti, "A novel approach to nonperturbative renormalization of singlet and nonsinglet lattice operators", Physics Letters B740 (2014) 30.

7. P. E. Shanahan, R. Horsley, Y. Nakamura, D. Pleiter, P. E. L. Rakow, G. Schierholz, H. Stüben, A. W. Thomas, R. D. Young, and J. M. Zanotti (CSSM and QCDSF/UKQCD Collaborations), "Determination of the strange nucleon form factors", Physical Review Letters 114 (2015) 091802.
8. Yuya Shimizu and Yoshinobu Kuramashi, "Critical behavior of the lattice Schwinger model with a topological term at $\theta = \pi$ using the Grassmann tensor renormalization group", Physical Review D90 (2014) 014508.
9. Yuya Shimizu and Yoshinobu Kuramashi, "Grassmann tensor renormalization group approach to one-flavor lattice Schwinger model", Physical Review D90 (2014) 074503.
10. H. Suno, Y. Suzuki, and P. Descouvemont, "Triple-α continuum structure and Hoyle resonance of ^{12}C using the hyperspherical slow variable discretization", Physical Review C91 (2015) 014004.
11. H. Suno and B. D. Esry, "Cold elastic and reactive atom-molecule collisions in helium−helium−alkali-metal triatomic systems", Physical Review A89 (2014) 052701.
12. Takeshi Yamazaki, Ken-ichi Ishikawa, Yoshinobu Kuramashi, and Akira Ukawa "Study of quark mass dependence of binding energy for light nuclei in 2+1 flavor lattice QCD", arXiv:1502.04182 [hep-lat].
13. Shinji Takeda and Yusuke Yoshimura, "Grassmann tensor renormalization group for one-flavor lattice Gross-Neveu model with finite chemical potential", Progress of Theoretical and Experimental Physics (2015) 043B01.

(2) Conference Papers

1. Y. Nakamura, X.-Y. Jin, Y. Kuramashi, S. Takeda, and A. Ukawa, "Update on the critical endpoint of the finite temperature phase transition for three flavor QCD with clover type fermions", Proceedings of Science (LATTICE2014) 194.
2. R. Horsley, J. Najjar, Y. Nakamura, H. Perlt, D. Pleiter, P.E.L. Rakow, G. Schierholz, A. Schiller, H. Stüben, and J.M. Zanotti, "Determining Sigma - Lambda mixing", Proceedings of Science (LATTICE2014) 110.
3. A. Chambers, R. Horsley, Y. Nakamura, H. Perlt, D. Pleiter, P.E.L. Rakow, G. Schierholz, A. Schiller, H. Stuben and R.D. Young, and J. Zanotti, "Connected and disconnected quark contributions to hadron spin", Proceedings of Science (LATTICE2014) 165.
4. X.-Y. Jin, Y. Kuramashi, Y. Nakamura, S. Takeda, and A. Ukawa, "Scalar correlators near the 3-flavor thermal critical point", Proceedings of Science (LATTICE2014) 195.
5. Takeshi Yamazaki, "Hadronic Interactions", Proceedings of Science (LATTICE2014) 009.
6. S. Takeda, X-Y. Jin, Y. Kuramashi, Y. Nakamura, and A. Ukawa, "Critical end point in Nf=3 QCD with finite density and temperature", Proceedings of Science (LATTICE2014)

196.

(3) Invited Talks

1. Y. Kuramashi, "Lattice QCD", US/Japan Exascale Applications Workshop, Gatlinburg, Tennessee, USA, Sep. 5-6, 2015.
2. Y. Kuramashi, "2+1 Flavor Lattice QCD Simulation on K Computer" CCS-BNL Workshop on Lattice Gauge Theories 2015 (CCS-BNL LGT 2015), University of Tsukuba, Tsukuba, Japan, March 12-13, 2015.
3. Y. Nakamura, "Critical endpoint of finite temperature phase transition for three flavor QCD" CCS-BNL Workshop on Lattice Gauge Theories 2015 (CCS-BNL LGT 2015), University of Tsukuba, Tsukuba, Japan, March 12-13, 2015.
4. Yuya Shimizu, "Tensor Renormalization Group Study of Lattice Schwinger Model", Seminar at Kyushu University, Apr. 11, 2014.
5. Yuya Shimizu, "Tensor Renormalization Group Study of Lattice Schwinger Model", Seminar at Nagoya University, Jul. 8, 2014.
6. Yuya Shimizu, "Tensor Renormalization Group Study of Lattice Schwinger Model", Seminar at Osaka University, Jul. 15, 2014.
7. Yuya Shimizu, "Introduction to Grassmann Tensor Renormalization Group in Low-Dimensional Lattice Gauge Theory", Seminar at Okayama Institute for Quantum Physics, Aug. 6, 2014.
8. Yuya Shimizu, "Tensor Renormalization Group Approach to Lattice Gauge Theory", Seminar at University of Tsukuba, Nov. 7, 2014.
9. Takeshi Yamazaki, "Hadronic Interactions", 32nd International Symposium on Lattice Field Theory, Columbia University, New York, June 23-28 2014.
10. Takeshi Yamazaki, "Hadronic interaction and beyond standard model from lattice gauge theory", Progress in Particle Physics 2014, Kyoto University, Kyoto, July 28-August 1 2014.
11. Takeshi Yamazaki, "Light nuclei from lattice QCD", Advances and perspectives in computational nuclear physics, Hilton Waikoloa Village, Hawaii, October 5-7 2014.
12. Takeshi Yamazaki, "格子 QCD を用いた原子核直接計算", RCNP workshop on QCD を基礎とする核子多体系物理の理解, Osaka University, Osaka, December 19-20 2014.
13. Takeshi Yamazaki, "Light nuclei from lattice QCD", RIKEN BNL Research Center workshop on Multi-Hadron and Nonlocal Matrix Elements in Lattice QCD, Brookhaven National Laboratory, NY, February 5-6 2015.
14. Takeshi Yamazaki, "格子 QCD を用いた軽い原子核の計算", 素粒子・原子核・宇宙「京からポスト京に向けて」シンポジウム, Kioi forum, Tokyo, March 11-12 2015.

15. Shinji Takeda, "Curvature of critical line in m_π-μ plane for 3-flavor QCD", CCS-BNL Workshop on Lattice Gauge Theories 2015 (CCS-BNL LGT 2015), University of Tsukuba, Tsukuba, Japan, March 12-13, 2015.

(4) Posters and presentations

1. Y. Nakamura, "Update on the critical endpoint of the finite temperature phase transition for three flavor QCD with clover type fermion" (talk), 32nd International Symposium on Lattice Field Theory (LATTICE 2014), Columbia University, Jun. 23-28, 2014.
2. Y. Nakamura, "The critical end-point of the finite temperature phase transition in three flavor QCD" (talk), XQCD14, June 19–21, 2014, Stony Brook University, New York, USA.
3. H. Suno, Y. Suzuki, and P. Descouvemont, "Triple-α continuum structure and Hoyle resonance of 12C using the hyperspherical slow variable discretization" (talk), 2015 Annual Meeting of the Physical Society of Japan, Waseda University, Tokyo, Japan, March 21-24, 2015.
4. H. Suno, Y. Nakamura, K.-I. Ishikawa, and Y. Kuramashi, "Block BiCGSTAB for lattice QCD on the K computer" (poster), The 5th AICS International Symposium, RIKEN AICS, Kobe, Japan, December 8-9, 2014.
5. H. Suno, N. Sakumichi E. Hiyama, "Theoretical study of helium triatomic systems using hyperspherical coordinates" (talk), 2014 Autumn Meeting of the Physical Society of Japan, Chubu University, Kasugai, Japan, September 7-10, 2014.
6. X.-Y. Jin, "Scalar correlators near the 3-flavor thermal critical point" (talk), 32nd International Symposium on Lattice Field Theory (LATTICE 2014), Columbia University, Jun. 23-28, 2014.
7. Yuya Shimizu, "Grassmann Tensor Renormalization Group Study of Lattice QED with θ Term in Two Dimensions" (talk), 32nd International Symposium on Lattice Field Theory (LATTICE 2014), Columbia University, Jun. 23-28, 2014.
8. Yuya Shimizu, "Numerical Analysis of Lattice Schwinger Model Including θ Term Using Tensor Renormalization Group" (poster), Progress in Particle Physics 2014, Kyoto University, Kyoto, Jul. 28-Aug. 1, 2014.
9. Yuya Shimizu, "Numerical Analysis of Phase Structure of Two-Dimensional Lattice QED in θ Vacuum" (talk), 2014 Autumn Meeting of the Physical Society of Japan, Saga University, Sep. 18-21, 2014.
10. Shinji Takeda, " Critical end point in Nf=3 QCD with finite density and temperature" (talk), 32nd International Symposium on Lattice Field Theory (LATTICE 2014), Columbia University, Jun. 23-28, 2014.

11. Takeshi Yamazaki, "Light nuclei from 2+1 flavor lattice QCD" (talk), Hadrons and Hadron Interactions in QCD 2015, Kyoto University, Kyoto, February 15-March 21 2015.

(5) Patents and Deliverables

1. H. Suno, Y. Nakamura, K.-I. Ishikawa, and Y. Kuramashi, "Block BiCGStab for lattice QCD on the K computer", AICS Technical Report No. 2014-001.
2. H. Suno, Y. Nakamura, Y. Kuramashi, Y. Futamura, and T. Sakurai, "Optimization of matrix-vector multiplication for Real-Space Density Functional Theory Code on the K computer", AICS Technical Report No. 2014-002.
3. S. Takeda, Y. Kuramashi, and Y. Nakamura, "An efficient algorithm for the computation of the reduced determinant for Wilson-Dirac operator", AICS Technical Report No. 2015-001.

Discrete-Event Simulation Research Team

1. Team members

Nobuyasu Ito (Team Leader)
Hajime Inaoka(Research Scientist)
Yohsuke Murase(Research Scientist)
Yuta Asano (Postdoctoral Researcher)
Tetsuo Imai (Postdoctoral Researcher)
Takeshi Uchitane (Postdoctoral Researcher)
Shih-Chieh Wang (Postdosctoral Researcher)
Tomio Kamada (Guest Researcher)

2. Research Activities

As computer performance grow, simulation models tend to become the more complex, and models have the more parameters and show complicated behavior. This often increase the number of simulation jobs, and analyses and visualizations of simulation results also become diversified. Each simulation and each analysis will be properly processed by computers if they are specified correctly, but error will easily be introduced by human side. In this sense, supercomputers are demanding not only greater programming skill but also more reliable operation and smarter decision of simulation parameters. To help the latter, the OACIS(**O**rganizing **A**ssistant for **C**omprehensive and **I**nteractive **S**imulations), a job management tool for simulations and analyses are designed and developped in the Discrete-Event Simulation Research Team(DESRT). It is coded 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. The first version was released in this year, and cultivation of its user group was started.

Partitioned global address space(PGAS) is an idea to treat memory space managed in each node of massive parallel computer like the K computer as a shared memory computer, which makes programming easier and simpler. A PGAS language named X10[1] is implemented to the K computer. In addition to the C++ version(so-called the native version) of X10 which were available already, Java version(so-callled the managed version) was implemented in this year.

Most simulation models can be formulated as evolutions on certain graphs. For example,

particle-dynamics and molecular-dynamics simulations usually update a system configuration using so-called pair lists and neighbor tables, lists of interacting agents, that is, particles or molecules, with each agent[2]. The pair lists define a graph in agents. The graph evolves with motion of agents and agents evolve on the graph, and it is in an opposite extreme of simulation models with so-called a stencil computation algorithm. Stencil computation is on regular lattices, but dynamic and complex graphs are to be a main target of DESRT. Complicated graphs demand additional efforts when we implement on computers: optimization of pipeline, memory and cache, and massive-parallel communications are demanding. So algorithm and coding technology of graph and network simulations and analyses have been studied in DESRT. In this year, automobile traffic which use a graph of road map and treat car agents on it, epidemic propagation which use a graph of human mobility and treat human interactions on it, and graph of social relation were targets.

Accurate observations and high resolution measurements are important to decide simulation parameters, but they are not always available. We can design them appropriately for natural-scientific phenomena, but they are difficult for social-scientific phenomena. All data of human activities in real society do not mean sufficient, but data of many repetitions for various social parameters and systems in various environments with various conditions are necessary in the sense of natural science with Francis Bacon's *"Novum Organum"* style. In this sense, social-scientific models and their simulations are challenging: *Idola* will be everywhere because each of us have one's understandings, interests and perspective about our society. So-called the "Big data" are far-from sufficient, which will intuitively obvious when the data size is compared with natural-scientific data, for example, data flood from modern accelerators and space telescopes. Such situation of data lack, theoretical studies are advantageous, and computer simulations are major driving force of theoretical challenge nowadays. Make models of cloudy target phenomena, examine their behavior precisely, and compare the clear behavior with vague target data to assess the models. This year, a simulation model of automobile traffic flow in Kobe city is analyzed with the standard factor analysis of multivariate statistical analysis. The model is agent-base one simulating motion of each car agent, and only coarse-grained data are adjusted to the real traffic. Estimated factors are reasonably explain what we are experiencing in our daily urban lives.

[1] http://x10-lang.org/

[2] Details of a molecular-dynamics simulation on K-type computers are given in, for example, Hiroshi Watanabe, Masaru Suzuki and Nobuyasu Ito, Computer Physics Communications 184 (2013) 2775, which is available at

http://www.sciencedirect.com/science/article/pii/S187538921400279X.

3. Research Results and Achievements

3.1. The OACIS

First version of the OACIS(**O**rganizing **A**ssistant for **C**omprehensive and **I**nteractive **S**imulations)[2] is made open for public use in the beginning of this year on github site[3], and tutorial and user support activities are started[4]. Overview of the OACIS is explained in the Figure 1, and an example of user interface is shown in the Figure 2.

This OACIS version 1.xx.x is for single-user managing up to about millions of jobs operating. Beyond this number of job, job management operations requires too long even for a simple simulator with a few inputs and a few output. Multithreading in parallel machine is now necessary to go beyond this limitation, and an improvement using PGAS language X10 was on schedule. There are two kinds of X10. One is on C++ which is callled the "native version" and the other is on Java called the "managed version". The native version had been available on the K computer and Fujitsu FX10.

The managed version will be more useful for the extension of OACIS because it has the more powerful library useful for the purpose. In this year, the managed version is now implemented on the K computer and Fujitsu FX10 and extension of the OACIS beyond the limitation of job number will use this X10 managed version.

Implementation of the OACIS may not be easy for users without experience of Ruby and MongoDB. Some users want to implement the OACIS on their Windows machine. Some users committing several projects need to execute several OACIS in one computer. Virtual machine will help to solve these request, and a preliminary version of the OACIS in the Docker container[5] was developped and been testing in this year.

[3] https://github.com/crest-cassia/oacis

[4] https://groups.google.com/forum/#!forum/oacis-users

[5] https://www.docker.com/

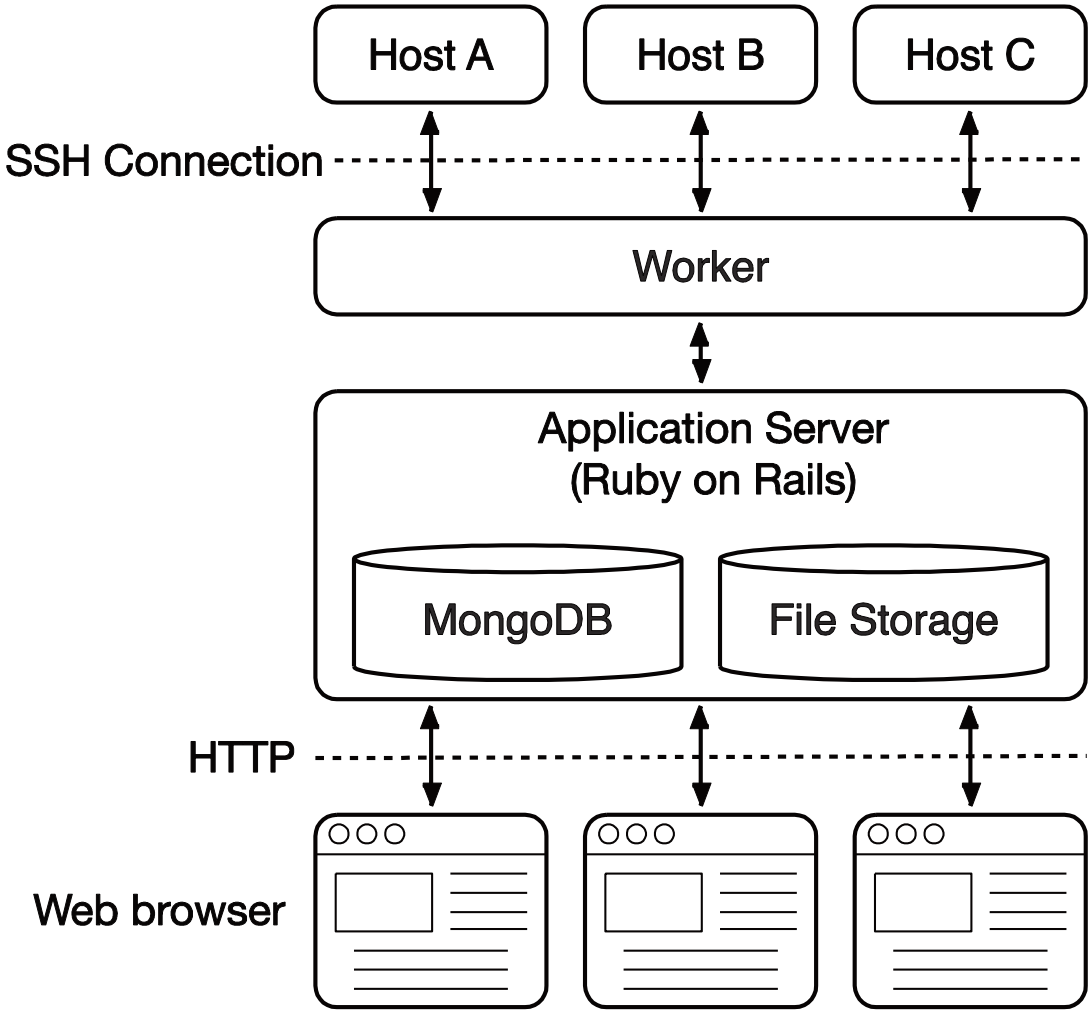
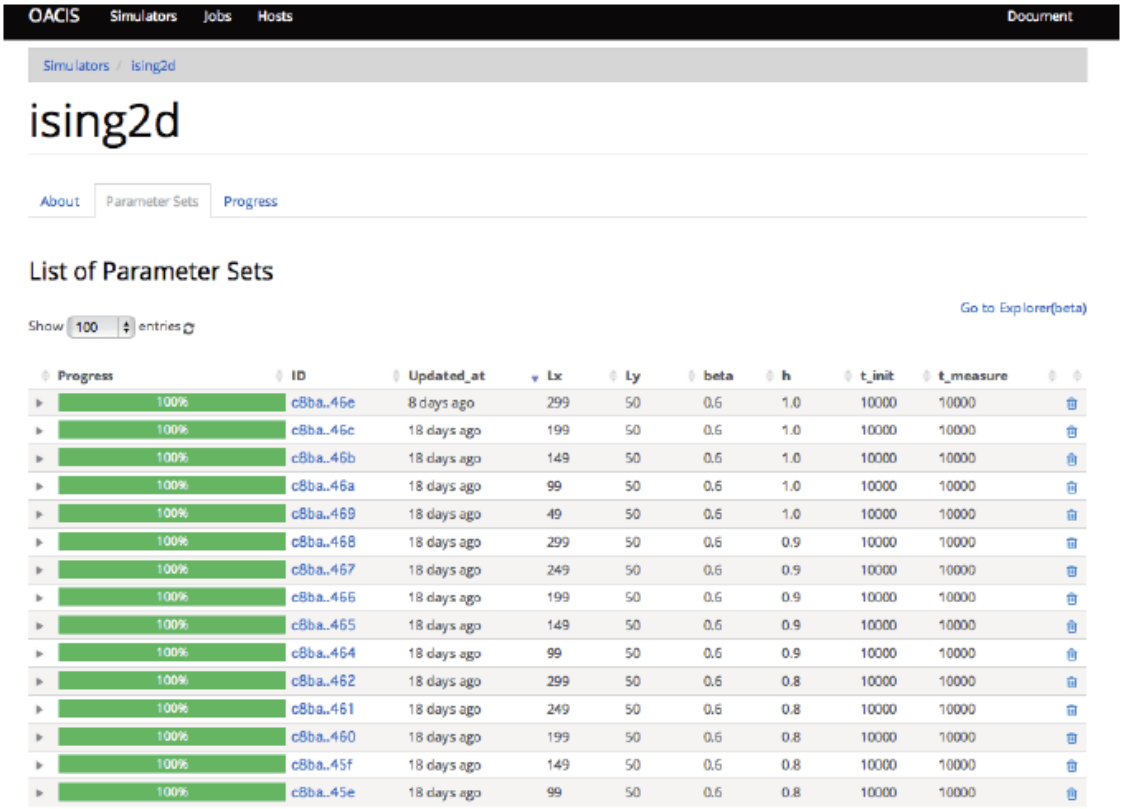


Figure 1. Overview of the OACIS is shown schematically[1]. The OACIS is between two horizontal broken lines. User in the bottom operates the OACIS through web browsers via HTTP. Host computers registered for job execution in the top are operated by the OACIS via SSH. The OACIS supports job executions on K-computer through K's standard staging, execution, and stage-out scheme.



Progress	ID	Updated_at	Lx	Ly	beta	h	t_init	t_measure
100%	c8ba..46e	8 days ago	299	50	0.6	1.0	10000	10000
100%	c8ba..46c	18 days ago	199	50	0.6	1.0	10000	10000
100%	c8ba..46b	18 days ago	149	50	0.6	1.0	10000	10000
100%	c8ba..46a	18 days ago	99	50	0.6	1.0	10000	10000
100%	c8ba..469	18 days ago	49	50	0.6	1.0	10000	10000
100%	c8ba..468	18 days ago	299	50	0.6	0.9	10000	10000
100%	c8ba..467	18 days ago	249	50	0.6	0.9	10000	10000
100%	c8ba..466	18 days ago	199	50	0.6	0.9	10000	10000
100%	c8ba..465	18 days ago	149	50	0.6	0.9	10000	10000
100%	c8ba..464	18 days ago	99	50	0.6	0.9	10000	10000
100%	c8ba..462	18 days ago	299	50	0.6	0.8	10000	10000
100%	c8ba..461	18 days ago	249	50	0.6	0.8	10000	10000
100%	c8ba..460	18 days ago	199	50	0.6	0.8	10000	10000
100%	c8ba..45f	18 days ago	149	50	0.6	0.8	10000	10000
100%	c8ba..45e	18 days ago	99	50	0.6	0.8	10000	10000

Figure 2. An example of snapshot of OACIS operation on a web browser is shown[1]. It browses status of specified jobs. A simulator named "ising2d" is prepared and registered on OACIS which execute a Monte Carlo simulation of the Ising model on square lattice with specified parameters: Lx, Ly, beta, h t_init and t_measure denoting lattice sizes in x and y directions, inverse temperature normalized by a spin-coupling constant, external field, number of Monte Carlo steps for initial relaxation and measurement, respectively. Each job is listed in a row.

3.2. Graph and network simulators

A benchmark program for the K computer aiming at car traffic simulation is made. Each car agent is driven at a given speed without interacting with any other cars, and it selects its way randomly at each corner. Geometrical parallelization is used: a given road network is divided into small areas geometrically, and each process on each computer node processes one of these small areas. Cars going out or coming into the area of each process are sent to or received from the process simulating corresponding areas.

Weak scaling of parallel performance was measured using a square-lattice road network(Figure 3). Lattice constant of this network corresponds to 100m, and each road segment has two lanes going to opposite direction with each other. Cars keep left lane. Initially, 16 cars are allocated par 100m of each lane. Velocity of each car is assigned uniformly randomly in a interval from 10Km/h to 60Km/h. Each node of the K computer processes area of 16×16, therefore totally 100m×16×16×2 lanes =51.2Km of lane per node, and 16×16×16×2=8192 cars in average per node. Time step Δt is 0.01sec and performance is measured for 1 million steps corresponding to 0.01sec$\times 10^6$ steps = 10^4 sec is measured. The results from 9 nodes with 3×3 to 20,736 nodes(quarter nodes of the K computer) with 144×144 are plotted in Figure 4. The processes on the smallest 9 nodes simulate 73,728 cars on totally 460.8Km lanes, and the performance was 9.5MUPS(million update per second) per node. The largest 20,736 nodes treat 169,869,312 cars on 1,061,683.2Km, and the performance was 7.2MUPS per node, which is 24% slower than 9 nodes.

Strong scaling of parallel perfornace is measured using both the Japanese road network and the square-lattice network. The Japanese road network is based on the Open Street Map[6] and totally 1,310,000Km and 127,000,000 cars are simulated on the map(See Figure 5). The square-lattice network with the corresponding total length and number of cars is also used. This number of cars should be compared with 77,193,872, the number of car in Japan in the end of September 2014. Time step Δt is 0.01sec and performance is measured for 1 million steps corresponding to 0.01sec $\times 10^6$ steps = 10^4 sec is measured. The performance with 324, 1,296, 5,184 and 20,736 nodes are plotted in Figure 6.

These results of strong scaling show peak around 5,184 nodes. Speed with 20,736 nodes is still faster than ones with 324 and 1,296 nodes. This will because the effect of cache memory. The speed of the Japanese traffic with 20,736 nodes was faster than 0.3MUPS per CPU core. And 0.3MUPS core will reasonably be expected when all nodes of the K computer is used which is 0.3MUPS×8 cores = 2.4MUPS per node, and 2.4MUPS×82.944 nodes = 0.20 TUPS(10^{12} UPS). This is a performance achieving a real-time simulation of two billion cars with Δt = 0.01 sec.

This is the performace with simplified car agents, each of which randomly moves around on the road network without interacting with other agents. In the more realistic model, car movement

costs more calculations in each computer nodes. Therefore weight of communication between nodes becomes less. So parallelization of traffic simulation on the K computer will work efficiently if parallelized loads are well-balanced.

In summary, the benchmark results will imply that the K computer can achieve a real time or faster simulation of all the car traffic in Japan.

[6] https://openstreetmap.jp/

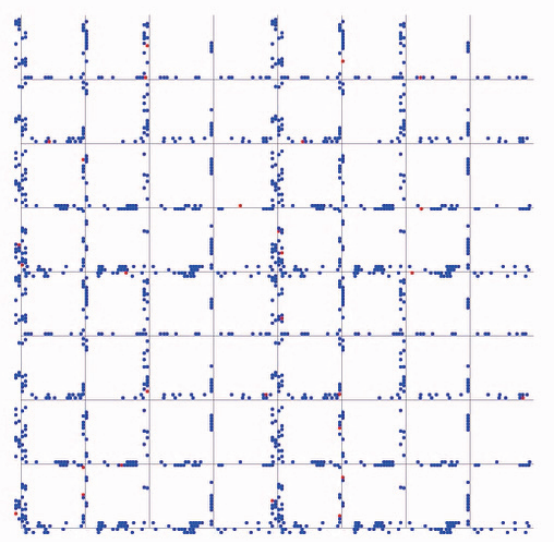


Figure 3: Traffic on the square-lattice road network is shown. Some segments have two traffic lanes for one direction on this figure, but the network for benchmark comprises one lane for each direction for all segments.

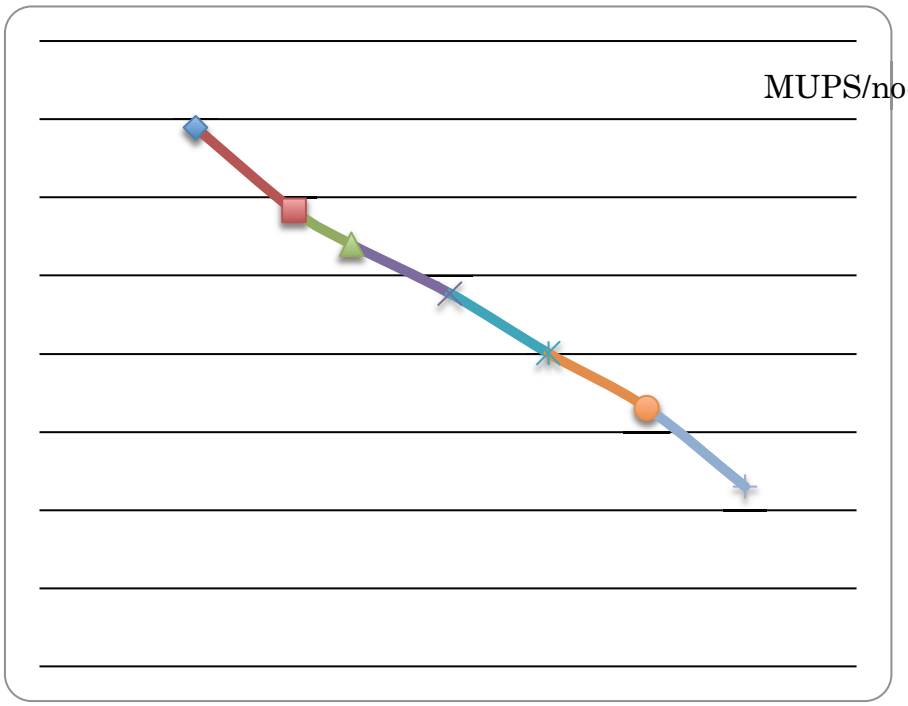
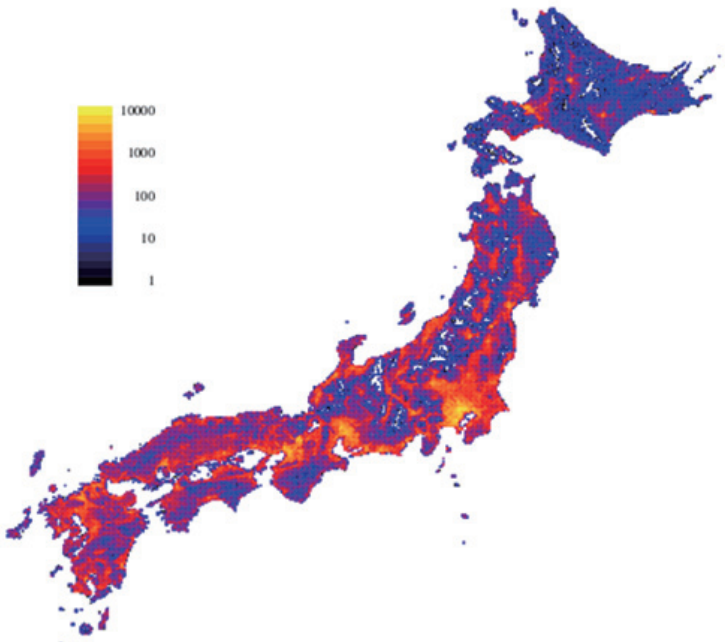


Figure 4: Weak-scaling performance results using square-lattice road network are plotted. The horizontal axis shows number of nodes and the vertical axis shows performance measured by number of cars updated on each node per second with a unit of million. "MUPS" is an abbreviation for "million updates per second".



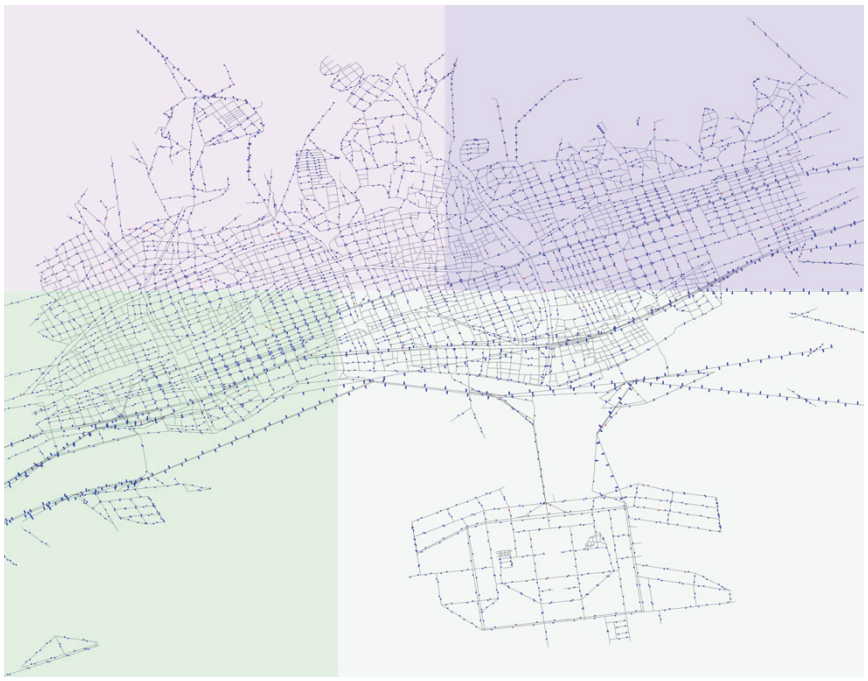


Figure 5: The Japanese road network used to evaluated the strong-scaling performance in Figure 6 is shown. Top: the network is visualized with density of crossing. Bottom: magnified snap-shot focused at the Kobe city.

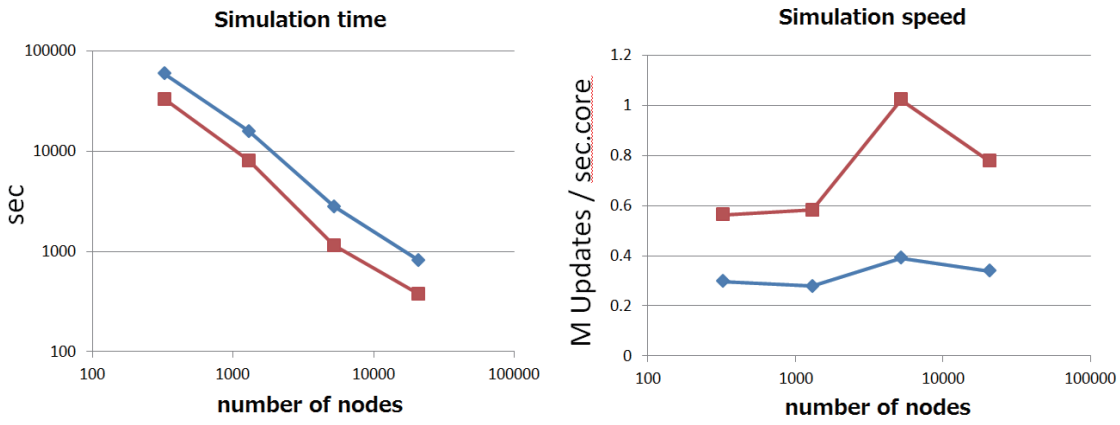


Figure 6: Results of strong-scaling parallel performance are plotted. Blue diamond denotes the results with the Japanese road network, and red square with the square-lattice network. Left:

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 developped. And a graph simulation and analysis tool working on K-computer up to its full node will be developped.

5. Publication, Presentation and Deliverables

(1) Journal Papers

1. Yohsuke Murase, János Török, Hang-Hyun Jo, Kimmo Kaski, János Kertész, "Multilayer weighted social network model", Physical Review E, vol.90 (2014) 052810.
2. Hiroshi Watanabe, Masaru Suzuki, Hajime Inaoka, and Nobuyasu Ito, "Ostwald ripening in multiple-bubble nuclei", Journal of Chemical Physics, vol.141 (2014) 234703.

(2) Conference Papers

1. Yohsuke Murase, Takeshi Uchitane, and Nobuyasu Ito, "A tool for parameter-space exploration"、Physics Procedia 57 (2014) pp. 73-76.

(3) Invited Talks

1. Nobuyasu Ito, "Simulation study of liquid-gas transition", International Conference "Smart functional materials for shaping our future" (Debrecen, Hungary, 19-20 September 2014) .

(4) Posters and presentations

1. Hiroshi Watanabe, Masaru Suzuki, Hajime Inaoka, and Nobuyasu Ito, "Huge-Scale Molecular Dynamics Simulation of Multi-Bubble Nuclei", NCSA Blue Waters Symposium for Petascale Science and Beyond(Champaign, Illinois, USA, May 2014).
2. Hajime Inaoka and Nobuyasu Ito, "Implementation of a breadth-first search algorithm on a massive-parallel computer", Social Modeling and Simulation + Econophysics Colloquim 2014, (Kobe, Japan, Nov. 2014),.
3. Yuta Asano, Nobuyasu Ito, Hajime Inaoka, Yohsuke Murase, Tetsuo Imai, and Takeshi Uchitane, "Traffic Simulation of Kobe-city", Social Modeling and Simulation + Econophysics Colloquim 2014, (Kobe, Japan, Nov. 2014).
4. Takeshi Uchitane, "A software for managing a lot of jobs and their results", Social Modeling and Simulation + Econophysics Colloquim 2014, (Kobe, Japan, Nov. 2014).
5. Yohsuke Murase, et al.“A Universal Lifetime Distribution for Multi-Species Systems”, Social Modeling and Simulation + Econophysics Colloquium 2014, (Kobe, Japan, Nov. 2014)
6. Yohsuke Murase, et al.“Multilayer weighted social network model”Social Modeling and Simulation + Econophysics Colloquium 2014, (Kobe, Japan, Nov. 2014), awarded as the Best Poster Prize
7. Hajime Inaoka and Nobuyasu Ito, "Molecular Dynamics Simulation of Pool Boiling of a Lennard-Jones Liquid", International Symposium on Extended Molecular Dynamics and Enhanced Sampling Nosé Dynamics 30 Years(Keio University, Tokyo, Japan, Nov. 2014).

8. Yohsuke Murase,et al. “Multilayer weighted social network model”, 5th AICS International Symposium.
9. Takeshi Uchitane, “OACIS - A tool for social simulation execution and its applications", The 5th AICS Symposium, 2014.

(5) Patents and Deliverables

OACIS, a job management application, released on April 1st, 2014.

Computational Molecular Science Research Team

1. Team members

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

2. Research Activities

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

2.1. Original molecular science theory to explore 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. 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.

2.2. New molecular science software NTChem

Quantum chemistry software comprises immensely useful tools in material and biological science

research. Widely diverse programs have been developed in Western countries as Japan has lagged. In fact, only a few programs have been developed in Japan. The mission of our research team is to provide K computer users with a high-performance software for quantum molecular simulation. In the early stage of the K computer project, no quantum chemistry software was available for general purpose and massively parallel computation on the K computer because not every program was designed for use on it. Therefore, we have chosen to develop a new comprehensive ab initio quantum chemistry software locally: NTChem. NTChem is completely new software that implements not only standard quantum chemistry approaches, but also original and improved theoretical methods that we have developed in our research work. The main features of the current version, NTChem2013, are the following:

1) Electronic structure calculation of the ground state of atoms and molecules based on Hartree–Fock (HF) and density functional theory (DFT) methods.

2) Linear-scaling or low-scaling DFT: Gaussian and finite-element Coulomb (GFC) resolution-of-the-identity (RI) DFT, pseudospectral DFT/HF, and dual-level DFT.

3) Low-scaling SCF calculation using diagonalization-free approaches: purification density matrix, pseudo-diagonalization, and quadratic convergence SCF.

4) Excited-state DFT calculation: time-dependent DFT (TDDFT) and transition potential (DFT-TP).

5) Accurate electron correlation methods for ground and excited states: Møller–Plesset perturbation theory, coupled-cluster (CC) theory, and quantum Monte Carlo (QMC) method.

6) Massively parallel computing on the K computer and Intel-based architectures: HF, DFT, resolution-of-the-identity second-order Møller–Plesset (RI-MP2) method, and QMC method.

7) Two-component relativistic electronic structure calculation with spin–orbit interactions: Douglas–Kroll (DK) (DK1, DK2, and DK3), regular approximation (RA) (zeroth-order RA (ZORA) and infinite-order RA (IORA)), and Relativistic scheme for Eliminating Small Components (RESC).

8) Model calculations for large molecular systems: quantum mechanics/molecular mechanics (QM/MM) and Our own N-layered Integrated molecular Orbital and molecular Mechanics (ONIOM).

9) Calculation of solvation effects: COnductor-like Screening MOdel (COSMO) (interfaced with the HONDO program), averaged solvent electrostatic potential/molecular dynamics (ASEP/MD), and QM/MM-MD.

10) Efficient calculation for chemical reaction pathway.

11) Ab initio molecular dynamics calculation.

12) Calculation of magnetic properties: nuclear magnetic resonance (NMR) chemical shifts, magnetizabilities, and electron paramagnetic resonance (EPR) g tensors.

13) Population analysis: Mulliken and natural bond orbital (NBO) analysis (interfaced with NBO 6.0).

14) Orbital interaction analysis: maximally interacting orbital (MIO) and paired interacting orbital (PIO) methods.

3. Research Results and Achievements

3.1. Development of massively parallel algorithm of RI-MP2 energy calculation and RI-MP2 analytical energy gradient calculation on peta-flops supercomputers

Second-order Møller–Plesset perturbation (MP2) theory is the simplest but robust electron correlation method to account for the non-covalent interactions that play important roles in the chemical phenomena of nano and biological molecules. In our previous study, we developed the MPI/OpenMP hybrid parallel algorithm (J. Chem. Theory Comput. 9, 5373 (2013)) for the resolution of the identity MP2 (RI-MP2) energy calculation of nano-scale molecules on peta-flops supercomputers and implemented into the NTChem software. However, it was difficult to perform the RI-MP2 calculations more than 10,000 MPI processes on the peta-scale supercomputers using the previously reported algorithm because it had the limitation of the available MPI processes.

We have developed the improved version of the MPI/OpenMP hybrid parallel algorithm for the RI-MP2 energy calculations. In this algorithm, we have developed the dual-level parallelization scheme to utilize more than 10,000 MPI processes on the peta-scale supercomputers such as the K computer and TSUBAME 2.5. We have also devised the network communication scheme overlapping the computation and the network communication during the evaluation of four-center two-electron repulsion integrals to reduce the overhead and the latency of network communication. We checked the scalability of parallel algorithm performing test calculations of nanographene stacked dimer $(C_{150}H_{30})_2$ at the RI-MP2/cc-pVTZ level (9,840 atomic orbitals (AOs) without the frozen core approximation) using up to 80,199 nodes of the K computer. The parallel performance scales up to the 80,199 nodes and the 3.1 peta FLoating OPerations per second (FLOPs) of peak performance has been attained using 80,199 nodes. We have performed the multi-node and multi-graphic processing unit (GPU) implementation based on the present algorithm. The DGEMM matrix–matrix multiplication during the RI-MP2 calculation is offloaded to the GPU devices. The dual-level parallelization scheme is also suitable for utilizing the multi-nodes and multi-GPUs where the computation of sub-matrices is assigned to each GPUs. Considerable speedups of the RI-MP2 calculation can be attained by the present multi-node and multi-GPU implementation. The peak performance of the central processing unit (CPU) computation and the CPU/GPU hybrid computation of nanographene stacked dimer $(C_{96}H_{24})_2$ (9,840 atomic orbitals (AOs) without the frozen core approximation) using 1,349 nodes and 4,047 GPUs of TSUBAME 2.5 are 87.5 tera FLOPs and 514.7 tera FLOPs, respectively.

In the case of geometry optimization, the MP2 analytical energy gradient calculation is more demanding than the MP2 energy calculation because of the high computational cost with very large

prefactors. Thus, the efficient computational algorithm and implementation for the MP2 energy gradient is desired. We have developed an MPI/OpenMP hybrid parallel algorithm for the RI-MP2 energy gradient calculation of nano-scale molecules and implemented into the NTChem software. This algorithm is designed for the massively parallel calculations on the peta-flop supercomputers such as the K computer. The loop of a virtual molecular orbital index is parallelized by MPI in the calculation of two-electron integrals, one-particle density matrices, and two-particle density matrices to utilize more than a few thousand MPI processes. The dual-level parallelization scheme and the network communication scheme overlapping the computation and network communication mentioned above have also been applied to the RI-MP2 energy gradient algorithm. The RI-MP2/cc-pVTZ energy gradient calculation of buckycatcher $C_{60}@C_{60}H_{28}$ (3,992 AOs without the frozen core approximation) was successfully performed in 30 minutes using 4,096 nodes of the K computer. Using the new MPI/OpenMP hybrid parallel RI-MP2 energy gradient code, the MP2 geometry optimization of large molecules having up to 200 atoms and 5,000 AOs can be performed with high parallel performance and in modest time on the K computer.

3.2. Development of higher-order time-dependent density functional theory for nonlinear optical properties

Molecular materials exhibiting large second-order nonlinear optical (NLO) responses have received increasing interest in recent years, experimentally as well as theoretically owing to their applicability in fields such as noninvasive imaging, three-dimensional optical data storage and optical power limiting. Correct description of excited states involved in NLO responses frequently requires inclusion of the higher order electronic correlations. This makes their computing a much more complicated procedure compared to analogous ground state calculations. Recently, time-dependent density functional theory (TDDFT) has emerged as an accurate and efficient method for studying the optical response of molecules. Including the electron correlation through the exchange–correlation functional, excellent results have been obtained for organic molecules, organometallic compounds, inorganic finite clusters, and infinite crystals.

In this work, we have implemented dynamic linear-, quadratic-, and cubic-response TDDFT method for nonlinear optical response of molecules in the NTChem program. The implemented code can calculate the typical nonlinear optical properties such as electrooptic Pockels effect (EOPE), second harmonic generation (SHG), optical rec- tification (OR), DC-electric field induced (EFI)SHG, third harmonic generation (THG), optical Kerr effect (OKE), and intensity dependent refractive index (IDRI). Those implementations closely follow the algorithm presented by Sekino and Bartlett for higher-order time-dependent Hartree–Fock theory. Higher-order Kohn–Sham matrices of higher-order Kohn–Sham equations require higher-order functional derivatives of the exchange–correlation functionals, which have been derived and implemented into efficient computer codes

with the aid of a computerized symbolic algebra system.

3.3. Development of screened Hartree–Fock exchange potential using position-dependent atomic dielectric constants

Screening effects on the exchange potential have been gathering a lot of attentions in first-principles band structure calculations. The importance of the screened exchange term has been discussed in the GW method and the COHSEX approximation, which was proposed by Hedin in 1965. One of important characteristics of the GW method is to improve the bandgap property of semiconductors, although the local density approximation (LDA) of density functional theory (DFT) underestimates the bandgap due to the lack of nonlocal exchange interactions. In the static COHSEX approximation of the GW method, electron correlation effects related to the random phase approximation (RPA) are divided into two contributions of the Coulomb-hole (COH) and the screened exchange (SEX) interactions. The non-local SEX contribution is essential to improve the bandgap problem of the LDA method. The hybrid DFT functionals which possess a partial Hartree–Fock (HF) exchange term can also give better agreements between calculations and experiments. Thus, the GW and hybrid-DFT methods can provide good solutions for the bandgap problem. Several studies have pointed out theoretical relationships between the GW method and the hybrid-DFT functionals. We developed a dielectric-dependent screened HF exchange potential approach and the dielectric-dependent Slater-formula and COH interaction. In the dielectric-dependent screened exchange approach, the ratio of the HF exchange term mixed into screened exchange potential is proportional to the inverse of the dielectric constant. In addition, we studied the screened HF exchange potential using position-dependent atomic dielectric constants. The estimations of the atomic dielectric constant are incorporated into the SCF loop, and those values are automatically determined in each SCF step. In order to confirm the adequacy of our position-dependent methodology, the energy band structures of several semiconductors are calculated, and the position-dependent approach can give good agreements with experimental results.

3.4. Development of computational scheme for natural circular dichroism

When lights have different degrees of circular polarization, they are absorbed differently by optically active chiral molecules. With no external magnetic field, this effect is called natural circular dichroism. Experimental circular dichroism spectroscopy has widely been used as a powerful tool to investigate structure of large molecules including protein, because of its sensitivity to the molecular conformation. In NTChem, we have implemented a functionality to investigate this natural circular dichroism, associated with electronic state excitations. In our implementation, both scalar and tensor rotational strength can be calculated in length or velocity representation. The conventional scalar rotational strength is relevant for light absorption by randomly oriented molecules, e.g., in gas-phase

or in solvent, whereas the tensor rotational strength is relevant for light absorption by oriented molecules, e.g., molecules adsorbed on surface. This new functionality is expected to be valuable calculational tool to interpret experimental results in circular dichroism spectroscopy.

3.5. Development of utility program for QM/MM combined calculation

For large systems such as proteins and supramolecules, fully quantum mechanical (full-QM) calculations are still too costly and some approximate approaches are required. Such approximate methods which combine accurate QM and less demanding molecular mechanical (MM) calculations are important portion of the NTChem program. However, to prepare NTChem input file for such multilevel calculations such as QM/MM and ONIOM calculations, are complicated and cumbersome. Thus, we developed a utility program for preparing QM/MM combined methods, which enables users to prepare input files for QM/MM calculations by using standard Tinker input and parameter files and indicating QM atoms. This utility program is written in Fortran90 and placed in NTChem tools packages.

3.6. Implementation of parallel algorithm for sparse-matrix algebra toward large-scale calculation of quantum chemistry

Recent development of computers has been making it possible to perform predictive calculations of electronic systems containing large molecules. For such calculations, we should employ linear-scaling methods, which are mainly used in the calculations based on the density functional theory (DFT). One of the most efficient methods for obtaining the ground state of a large electronic system is the purification method, in which the many multiplications of large sparse matrices are performed until convergence. The most crucial factor is thus the use of computationally as less demanding algorithm as possible for the multiplication of large sparse matrices. A promising algorithm for sparse-matrix algebra was proposed recently, in which a large sparse matrix is distributed to processors according to the density of the nonzero elements in the matrix and the multiplication between such matrices are efficiently performed using the communication. Specifically, a large matrix is divided into submatrices and their sparsity are determined in advance of multiplication. If the sparsity of two submatrices involved in the multiplication is dense, the ordinary matrix multiplication is performed. Otherwise, only the nonzero elements in the submatrices are sent and received for the multiplication. This treatment reduces the amount of data in the communications.

3.7. Theoretical design of dye sensitizers by two-component relativistic time-dependent density functional theory with spin–orbit interaction

Ru complexes have been demonstrated as a promising dye among solar cell materials. Recently, a

phosphine-coordinated Ru(II) sensitizer, DX1 molecule, was reported to perform well as an organic photovoltaic material. 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 DX1 sensitizer can absorb long-wavelength lights through the spin-forbidden transitions. Last year, we successfully reproduced the spin-forbidden transitions by two-component relativistic time-dependent density functional theory/ Tamm–Dancoff approximation with the SO interaction (2c-TDDFT/TDA), which was implemented into NTChem. This year, we newly examined the roles of the central transition metal by replacing Ru with Fe and Os. The numerical investigation reveals that the absorption spectrum of DX1–Fe is similar to that of DX1–Os but is significantly different. DX1–Os can absorb longer wavelength light with relatively small oscillator strengths in comparison with DX1, whereas DX1–Fe cannot. This investigation provides information about the roles of transition metals in dye sensitizers, which would be useful for constructing new sensitizers using spin-forbidden transitions.

3.8. Computational application to organic photovoltaics

Compared to the conventional silicon-based solar cells, organic photovoltaics (OPV) are characterized by their lower production costs, lower weights and greater flexibilities. In addition, OPV can be produced by printing on materials so that they are expected to be useful for electric power generation on complex shaped materials like household goods, furniture, textile, and so on. Despite significant research efforts, detailed understanding of microscopic processes in OPV is still lacking. Especially, the charge generation mechanism at the heterojunction between donor and acceptor has been debated for a while. To understand this process, we have investigated the properties excited electronic states in a P3HT:PCBM monomer pair, where P3HT is a popular donor polymer material and PCBM is an acceptor material derived from C_{60} fullerene, using the time-dependent DFT method. We calculated the electronic couplings for charge separation from the exciton at a P3HT monomer, and recombination from charge transfer state to the ground electronic state.

3.9. A computational estimation for orbital energies of polymer toward the development of organic photovoltaic cells

We theoretically investigated physical properties including orbital energies and excitation energies of frontier orbitals for the multifunctional thiophene-based polymers composed of donor- and acceptor-units. Orbital analysis reveals that the remarkably different behavior of frontier orbital energies with respect to the degree of the polymerization stems from the distributions of frontier orbitals, which is insightful information for controlling ionization potentials and electron affinities of multifunctional polymers. We also estimated frontier orbital energies of the polymers through a

simple Hückel-theory based analytical model parameterized from calculations of relatively small oligomers. In this model, we set two parameters: one is the orbital energy of each monomer α and the other is interaction energy corresponding to the resonance integral ß. Assumed that the resonance integral ß is proportional to the density of the edge atom connected to the next monomer, the orbital energy of a polymer can be estimated by its monomer. By using the fitted parameter, the estimated value from the data of a monomer can reproduce the orbital energy of the polymer. These analyses are meaningful for a future design of thiophene-based polymers for solar cell materials; for instance, we can design a new polymer that absorbs important long wavelength sunlight so that the LUMO energies decrease with respect to the degree of the polymerization by controlling orbital energies of the donor and acceptor units in the polymer.

4. Schedule and Future Plan

In the next financial year, we will develop the new algorithm and improve the parallel efficiency of the NTChem2013 suit of program. In addition, we will make NTChem more user-friendly. Currently, NTChem is available on several cluster and supercomputer systems (the supercomputer system of Research Center for Computational Science at the Institute for Molecular Science and the supercomputer system of the Foundation for Computational Science) as well as the K computer. In the near future, we hope to make NTChem available to the general public. We intend to continue adopting users' requests with the aim of making the program more convenient and user-friendly for researchers in various fields. We earnestly hope that NTChem will be an important tool leading the way toward a new frontier of computational molecular science.

5. Publication, Presentation and Deliverables

(1) Journal Papers

1. T. Nakajima, M. Katouda, M. Kamiya, Y. Nakatsuka, "NTChem: A high-performance software package for quantum molecular simulation", Int. J. Quantum Chem. 115, 349–359 (2015).
2. T. Nakajima, "Molecular science software "NTChem" and its application to complex systems", in Quantum and computational chemistry for metal complex systems (2014). (in Japanese)
3. T. Nakajima, "Douglas–Kroll method", Journal of Computer Chemistry, Japan, 13, 50‐70 (2014). (in Japanese)
4. T. Shimazaki, T. Nakajima, "Theoretical study of a screened Hartree-Fock exchange potential using position-dependent atomic dielectric constants", J. Chem. Phys., 142, 074109 (2015).
5. M. Shoji, H. Isobe, S. Yamanaka, Y. Umena, K. Kawakami, N. Kamiya, J.-R. Shen, T.

Nakajima, K. Yamaguchi, “Large Scale QM/MM Calculations of Oxygen Evolving Complex of Photosystem II. Elucidation of Hydrogen Bonding Networks for Proton Transfer and Water Inlet Channels for Water Oxidation”, Advances in Quantum Chemistry, 70, 325–413 (2015).

6. Y. Ootani, Y. Akinaga, T. Nakajima, “Theoretical Investigation of Enantioselectivity of Cage-Like Supramolecular Assembly: The Insights into the Shape Complementarity and Host–Guest Interaction”, J. Comput. Chem. 36, 459–466 (2015).
7. M. Shoji, H. Isobe, S. Yamanaka, Y. Umena, K. Kawakami, N. Kamiya, J.-R. Shen, T. Nakajima, K. Yamaguchi, “Theoretical modelling of biomolecular systems I. Large-scale QM/MM calculations of hydrogen-bonding networks of the oxygen evolving complex of photosystem II”, Mol. Phys. 113, 359–384 (2015).
8. K. Sugahara, N. Satake, K. Kamata, T. Nakajima, N. Mizuno, “A Basic –7-Charged Germanodecatungstate Efficient for Chemoselective Acylation of Primary Alcohols”, Angew. Chem. Int. Ed. 126, 13464–13468 (2014).
9. T. Shimazaki, T. Nakajima, “Dielectric-dependent screened Hartree-Fock exchange potential and Slater-formula with Coulomb-hole interaction for energy band structure calculations”, J. Chem. Phys. 141, 114109 (2014).
10. K. Uehara, T. Miyachi, T. Nakajima, N. Mizuno, “Effects of heteroatoms on electronic states of divanadium-substituted γ-Keggin-type polyoxometalates”, Inorg. Chem. 53, 3907–3918 (2014).
11. T. Shimazaki, T. Kosugi, T. Nakajima, “Range-Separation Density-Fitting Band Structure Calculation with Gaussian Auxiliary Function”, J. Phys. Soc. Jan, 83, 054702 (6 Pages) (2014).
12. 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 CeO2: Density Functional Calculation”, J. Chem. Phys., 140, 121102 (2014).
13. Y. Ikabata, Y. Tsukamoto, Y. Imamura, H. Nakai, “Local Response Dispersion Method in Periodic Systems: Implementation and Assessment”, J. Comput. Chem. 36, 303–311 (2015).
14. Y. Imamura, K. Suzuki, T. Iizuka, H. Nakai, “Linearity Condition for Orbital Energies in Density Functional Theory (V): Extension to Excited State Calculations”, Chem. Phys. Lett. 618, 30–36 (2015).
15. T. Baba, T. Matsui, K. Kamiya, M. Nakano, Y. Shigeta, “A density functional study on pKa of small polyprotic molecule”, International Journal of Quantum Chemistry, 114, 1128–1134 (2014).

(2) Conference Papers

(3) Invited Talks

1. T. Nakajima, “Catalysis design with NTChem”, 6th ESICB symposium, Tokyo, 18 March 2015. (in Japanese)
2. T. Nakajima, “Development of application software and co-design in post-K project”, 1st ft-energy symposium, Okazaki, 10 March 2015 (in Japanese)
3. T. Nakajima, “Molecular science software “NTChem” and drug design”, 2014 drug design informatics seminar, Tokyo, 17 December 2014 (in Japanese)
4. T. Nakajima, “Molecular science software “NTChem””, VINAS Users Conference 2014, Tokyo, 10 October 2014. (in Japanese)
5. T. Nakajima, “Simulation for organic film solar cell and photosynthesis”, 2nd TCCI informal meeting, Nagoya, 27 September 2014 (in Japanese)
6. T. Nakajima, “NTChem Program Package”, Current Topics in Theoretical Chemistry, Nha Trang Workshop 2014, Nha Trang, Viet Nam, 25 Aug. 2014.
7. T. Nakajima, “Post K project in AICS – molecular science –“, Post K seminar, Okazaki, 1 April 2014. (in Japanese)
8. M. Kamiya, T. Nakajima, “Development of Two-component Relativistic Time-dependent Density Functional Theory with Spin-orbit Interaction”, Second China-Japan-Korea Tripartite Workshop on Theoretical and Computational Chemistry (CJK-WTCC-II), Kobe (Japan) 23 Jan. 2015.
9. M. Katouda, “Algorithm and implementation of Møller–Plesset perturbation theory for petaflops supercomputers”, 4th International Workshop on Massively Parallel Programming Now in Quantum Chemistry and Physics - Toward post-K computers, Tokyo, 24 Nov. 2014.
10. T. Shimazaki, T. Nakajima, “Development of range-separation density-fitting approach for band structure calculations based on Gaussian basis set”, 18th Malaysian International Chemical Congress, Kuala Lumpur, Malaysia, 3 Nov. 2014.
11. Y. Imamura, “Theoretical Investigation on Dye Sensitizer Solar Cell: Spin-forbidden Transition”, 11th International Conference of Computational Methods in Sciences and Engineering (ICCMSE 2015), Athens (Greece), 20 Mar. 2015.
12. T. Matsui, “A novel computational scheme to estimate the redox potential of metal complex”, The 64th Conference of Japan Society of Coordination Chemistry, Tokyo, Japan, 18 September 2014.
13. M. Tashiro, "Molecular double core-hole state: theoretical analysis of photo- and Auger electron spectra", International Workshop “Atomic and molecular physics: a joint Japanese and French view over 120 years”, Cernay la Ville France, 21–23 July 2014.

(4) Posters and presentations

1. T. Matsui, J.-W. Song, K. Hirao, T. Nakajima, “Computational Scheme for Redox Potential with Long-range Corrected Density Functional Theory”, The 95th Annual meeting of Chemical Society of Japan, Funabashi, Japan, 29 March 2015.
2. M. Katouda, T. Nakajima, “Massively parallel RI-MP2 energy gradient algorithm for geometry optimization on petaflops supercomputers”, International Workshop on New Frontier of Numerical Methods for Many-Body Correlations―Methodologies and Algorithms for Fermion Many-Body Problems, Tokyo, 20 Feb. 2015. (Poster)
3. M. Katouda, T. Nakajima, “Massively parallel RI-MP2 energy gradient calculations on K computer”, 5th AICS International Symposium, Kobe, 8 Dec. 2014. (Poster)
4. M. Katouda, T. Nakajima, “MPI/OpenMP hybrid parallel algorithm of RI- MP2 energy gradient calculation for massively parallel multicore supercomputers”, QSCP-XIX, Taipei, 13 Nov. 2014. (Poster)
5. Y. Imamura, M. Kamiya, T. Nakajima, “Theoretical Study on Solar Cell Sensitizers by Two-component Relativistic Time-dependent Density Functional Theory”, the 19th International Workshop on Quantum Systems in Chemistry, Physics and Biology (QSCP-XIX), Taipei (Taiwan), 13 Nov. 2014.
6. M. Kamiya, H. Sekino, T. Nakajima, “Development of time-dependent density functional theory for frequency-dependent nonlinear optical response”, 8th Annual Meeting of Japan Society for Molecular Science, Kyoto, Japan, 24 September, 2014. (Poster)
7. Y. Imamura, M. Kamiya, T. Nakajima, “Theoretical Study on Design for Efficient Dye Sensitized Solar Cell Materials”, Annual Meeting of Japan Society for Molecular Science (2014), Higashi Hiroshima, 23 Sep. 2014.
8. Y. Imamura, M. Kamiya, T. Nakajima, “Theoretical Study on Photo Functional Materials by Two-component Relativistic Time-dependent Density Functional Theory”, 17th Theoretical Chemistry Symposium, Nagoya, 23 May 2014.

(5) Patents and Deliverables

Computational Materials Science Research Team

1. Team members

Seiji Yunoki (Team Leader)
Sandro Sorella (Senior Visiting Researcher)
Yuichi Otsuka (Research Scientist)
Shigetoshi Sota (Research Scientist)
Shixun Zhang (Postdoctoral Researcher)
Ahmad Ranjbar (Postdoctoral Researcher)
Keiko Matsuoka (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 Hubbard-type lattice models of interacting electrons. Typical target systems we aim are of the order of 10,000 electrons unless the notorious minus-sign problem occurs. One of the main focuses in our QMC project is to explore a possible quantum criticality in electron correlation driven quantum phase transitions.
2. We develop a massively parallel density matrix renormalization group (DMRG) algorithm for strongly correlated quantum systems. It is commonly accepted that the DMRG method is superior to investigate various properties in one-dimensional quantum systems. However, taking full advantage of huge computational resources such as the K computer, we can obtain highly accurate results in higher spatial dimensions. Our massively parallel DMRG algorithm can be used not only for typical quantum systems in condensed matter physics but also for molecules and bio-related materials in quantum chemistry by combining ab-initio first-principles calculations. Our DMRG algorithm can calculate static quantities as well as excitation dynamics (dynamical DMRG, DDMRG) and real time evolution of quantum states (time dependent DMRG, tDMRG).
3. We develop Monte Carlo (MC) and Molecular Dynamics (MD) simulation codes for large-scale classical spin systems for chiral magnets, which exhibit very rich phases due to the competition between e.g., Dzyaloshinskii–Moriya interaction and Zeeman interaction. The codes are implemented with capability to simulate over 2 million spins, which is made possible by our highly efficient and parallel algorithm. An important advantage of our codes is to be able to simulate large enough systems in three spatial dimensions, in which there exists many unanswered questions such as the fine grain spin structures of magnetic Skyrmion crystals and

the surface magnetic structures.

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 unprecedentedly large systems.

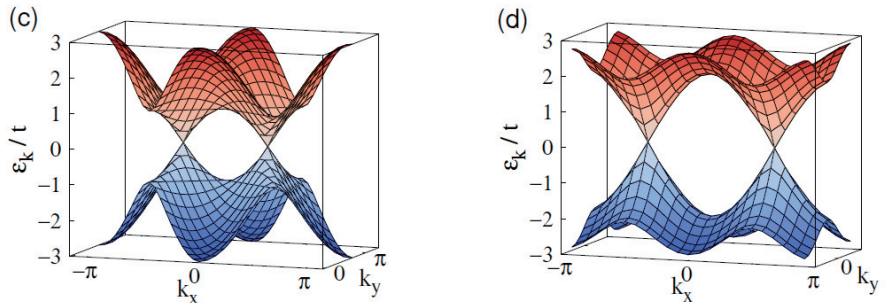


Fig. 1: Energy dispersions at U/t=0 (left: honeycomb, right: π-flux)

By using this improved code, we have clarified the nature of Mott transition in interacting Dirac fermions in two spatial dimensions. We have studied two different lattice models, the half-filled Hubbard model on the honeycomb lattice (honeycomb lattice model) and the half-filled Hubbard model on the square lattice with a magnetic flux π per plaquette (π-flux model), both of which have massless Dirac dispersions in the non-interacting limit with the Dirac point exactly at the Fermi level (Fig. 1). Due to this dispersion, the ground state of each model at weak coupling region is a semi-metal (SM), while it is expected to become the antiferromagnetic (AF) Mott insulator (MI) for strong coupling because of bipartiteness of the lattice structure. These Hubbard-type models with the Dirac dispersions have attracted much interest in the

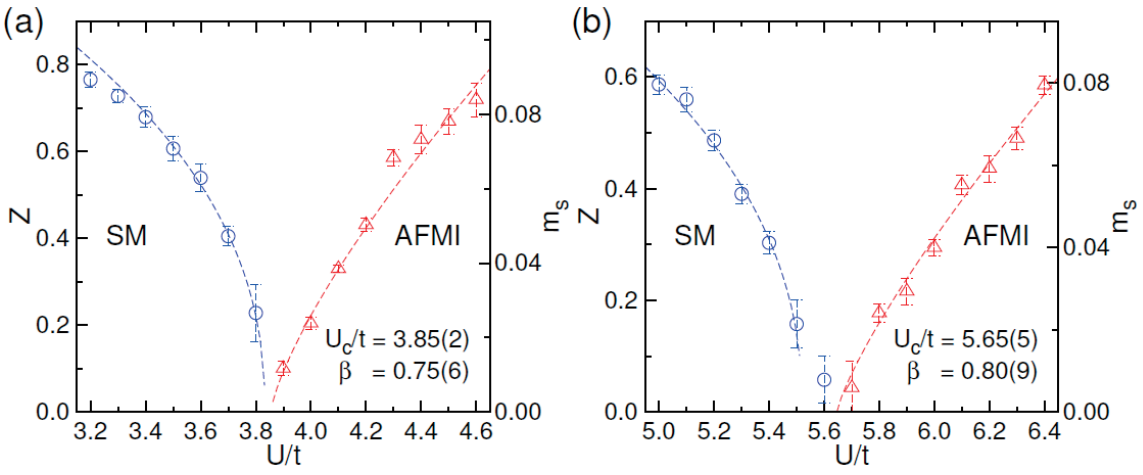


Fig. 2: The ground-state phase diagrams (left: honeycomb, right: π-flux).

field of the condensed matter physics soon after the proposal that there exists a spin-liquid (SL)

phase, a novel quantum state of matter, between SM and AFMI, which was first claimed in the honeycomb lattice model [Meng et al., Nature **464**, 847 (2010)] followed by a similar work in the π-flux model [Chang and Scalettar, Phys. Rev. Lett. **109**, 026404 (2012)]. It is, however, worth thinking carefully whether the SL phase can be possible without some geometrical frustration or peculiar interaction.

First, we have reexamined the ground state phase diagrams for both models by calculating order parameters for the Mott transition as a function of the Hubbard interaction (U/t). The results are summarized in Fig. 2. It is apparent in Fig.2 that the quasi-particle weight (Z), which is indicative of the metal-insulator transition, vanishes at the same point where the staggered magnetization (m_s) begins to develop. This clearly supports the conventional scenario that the Mott transition is direct and continuous from SM to AF; in other words the possibility of the SL phase is excluded. Having established the continuous character of the transition, we have performed careful finite-size scaling analysis to obtain critical exponents. As shown in Fig. 3, the data of the staggered magnetization calculated on finite-size clusters are satisfactorily collapsed into a universal function in each model, and it is turned out that the critical exponents are the same within the statistical errors for the two lattice models, which strongly suggests that the Mott transitions in these models belong to the same universality class. This class should be coincident with those observed in the Gross-Neveu model, a model extensively studied in the particle physics, since it has recently been recognized that the effective model for the interacting Dirac fermions in the continuous limit is described by the Gross-Neveu model. Thus, we expect that our finding based on the unbiased large-scale QMC simulations have an impact in interdisciplinary fields.

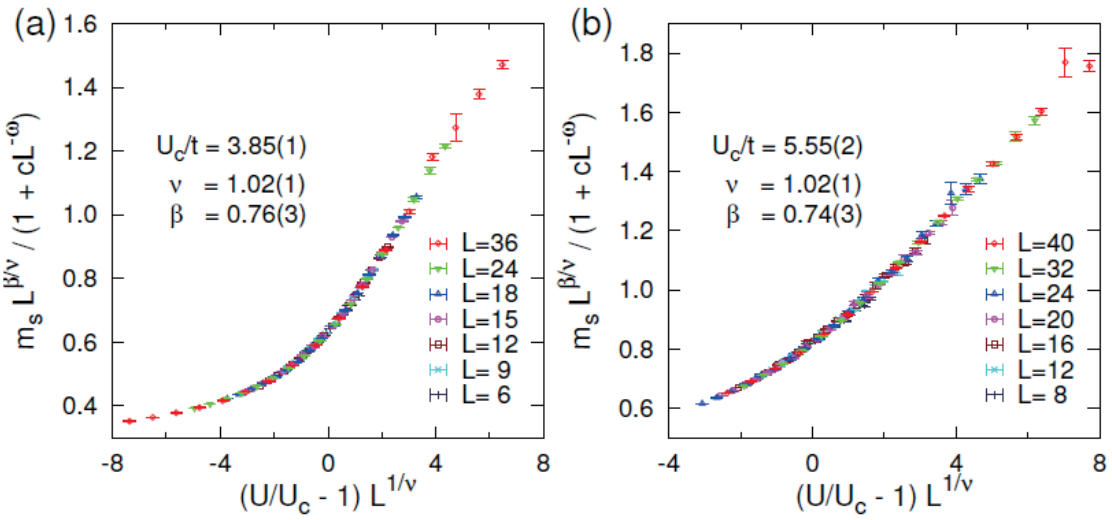


Fig. 3: Data collapse fits (left: honeycomb, right: π-flux) for different sizes L.

3.2. Development of massively parallelized two-dimensional (2D) DMRG algorithm and its applications

The DMRG method is known as one of the most powerful and accurate numerical methods for one-dimensional strongly correlated quantum systems. To the contrary, in two or higher spatial dimensions, the DMRG method is less accurate when the same computational resource is used because the number of truncation number m is required to be exponentially large in higher spatial dimensions than in one dimension in order to obtain the same numerical accuracy. Note that the DMRG truncation number m determines the computational costs because the dimension of matrix to be diagonalized is m^2. However, using huge computational resources available in the K computer, we can obtain highly accurate results for strongly correlated quantum systems even in higher spatial dimensions.

In this fiscal year, we have improved our 2D DMRG algorithm with additional functionalities. When a physical quantity is calculated, the DMRG procedure has to construct an operator corresponding to this physical quantity, using the renormalized basis set which is updated every DMRG iteration. The traditional DMRG algorithm thus must add a routine to do this transformation to each physical quantity. This is highly inconvenient for users, since physical quantities which can be calculated in our 2D DMRG code are limited. Thus, we have developed the DMRG algorithm, which can calculate any physical quantities without touching the source code. This algorithm is based on the idea to preserve the transformation matrix itself, but not each operator, and to construct operators from the transformation matrix when physical quantities are calculated. With this improved algorithm, users can now calculate any physical quantities. Also restoring transformation matrices after finishing the DMRG calculation, we can calculate physical quantities in separate jobs. This should be also important since the CPU time during which a single job can run is usually limited.

As one of the applications of our newly developed 2D DMRG algorithm, we have studied the ground state phase diagram of a quantum spin model for Na_2IrO_3, where the zigzag magnetic order is observed by neutron scattering experiments. The low-energy physics of Na_2IrO_3 has been believed to be effectively described by a quantum spin S=1/2 model with Kitaev-type interaction in addition to the isotropic Heisenberg interactions. However, it is turned out that the Kitaev-Heisenberg model cannot straightforwardly reproduce the zigzag type antiferromagnetic order as in experiments. Therefore, we have extended the Kitaev-Heisenberg model by including the next leading interactions and studied the ground state magnetic order. The model studied is described by the following Hamiltonian:

$$H = \sum_{(\alpha,\beta,\gamma)} \sum_{<lm>} KS_l^\gamma S_m^\gamma + J(S_l^\alpha S_m^\alpha + S_l^\beta S_m^\beta) + \tilde{I}_1(S_l^\alpha S_m^\beta + S_l^\beta S_m^\alpha) + \tilde{I}_2(S_l^\alpha S_m^\gamma + S_l^\gamma S_m^\alpha + S_l^\beta S_m^\gamma + S_l^\gamma S_m^\beta)$$

where $(\alpha, \beta, \gamma) = (x, y, z)$, (z, x, y) and (y, z, x), the S_l^α is the spin operator at the l-th site with α

component, and K, J, $\tilde{I}_1$, and $\tilde{I}_2$ are exchange interaction parameters between nearest neighboring spins. The ground state phase diagram is summarized in Fig. 4. We find that i) the zigzag magnetic order appears in a parameter regime relevant to Na_2IrO_3 and ii) there is the second order phase transition between the zigzag phase and the Kitaev spin liquid phase.

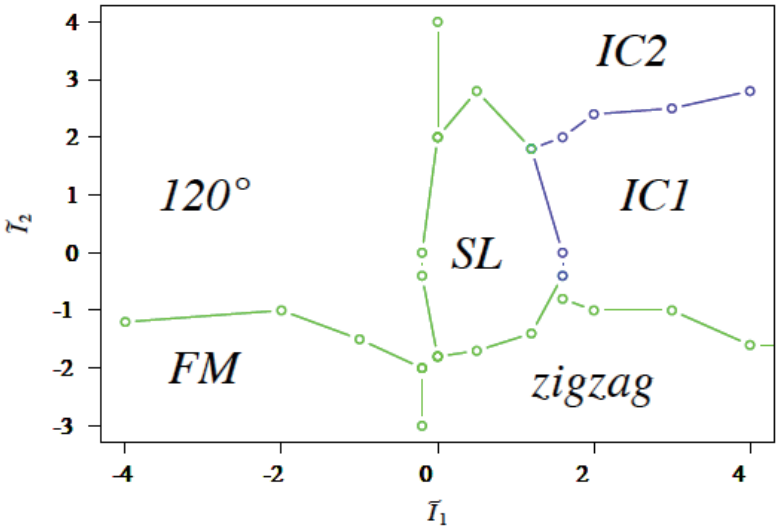


Fig. 4: The ground state phase diagram of the effective spin model for Na_2IrO_3. The unit of both axes is J. We set K = 20.0 meV and J = 0.8 meV.

3.3. Development of massively parallel DMRG algorithm for quantum chemistry

We have been developing a massively parallel DMRG algorithm for quantum chemistry to study electronic and magnetic properties of molecules and bio-related materials. Applying the techniques developed for our 2D DMRG, we have developed the massively parallel DMRG algorithm for quantum chemistry in order to perform highly accurate calculations for larger molecules. Compared with the case for strongly correlated quantum systems in condensed matter physics, the DMRG calculation in quantum chemistry requires huge memory size. This is simply because a Hamiltonian in quantum chemistry has usually many and usually long-ranged one and two-body terms, which are given by ab-initio calculations. If we use the straightforward extension of our DMRG algorithm to the quantum chemical systems, the memory usage becomes too large to handle because the memory requirement scales like O(N^5), where N is the number of orbitals, and thus we can only treat small number of orbitals even when the K computer is used. To overcome this difficulty, we have developed a new DMRG algorithm. In this new algorithm, we preserve the transformation matrix of the renormalized basis set, instead of operators themselves. The new algorithm reduces the memory usage significantly down to O(N), and construct each operator whenever it is needed during DMRG calculations. It should be emphasized that this algorithm does not require much additional computational time since the reduced density matrix can be block diagonalized in terms of conserved quantities such as charge and spin.

3.4. MC and MD simulations for chiral magnets

The schematic structure of our program modules is shown in Fig. 5. First, the program loads initial input data through "Data I/O" module and then pass it to "input parser" module to parse the input parameters. Using these prameters, the program constructs a model Hamitonian, which will be solved by MC and/or MD simualtion(s). Since MC and MD methods have their own pros and cons, here we conbine the two methods to make the simualtion more effcient. For example, for a given model, we start with a MC simulaiton to reach thermal equilbrum state followed by a MD simulation to eximine the stability of that spin structure and/or the time evolution. During these simulations, we can measure quantities such as spin configurations, energy, magneticzaiton and various correlation functions. These measurement data are finally stored into output file through "Data I/O" module. Moreover, we have implemented a set of tools for data post-processing and analysis. Data visualization is an important element to reveal spin configruations in real space. In the program, we use python combined with mayavi module to render spin configurations and time depedenet animations.

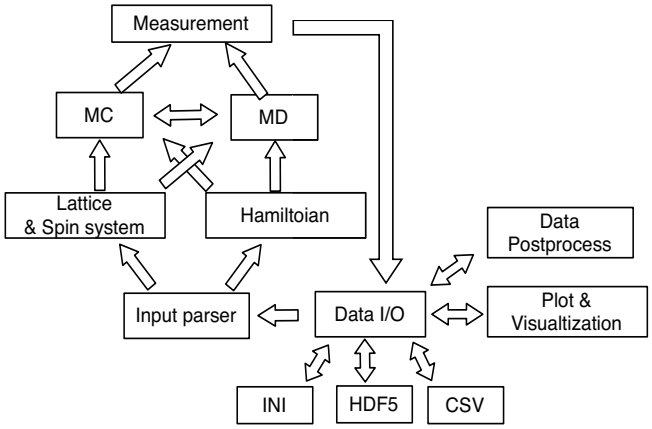


Fig. 5: Schematic diagram of program modules.

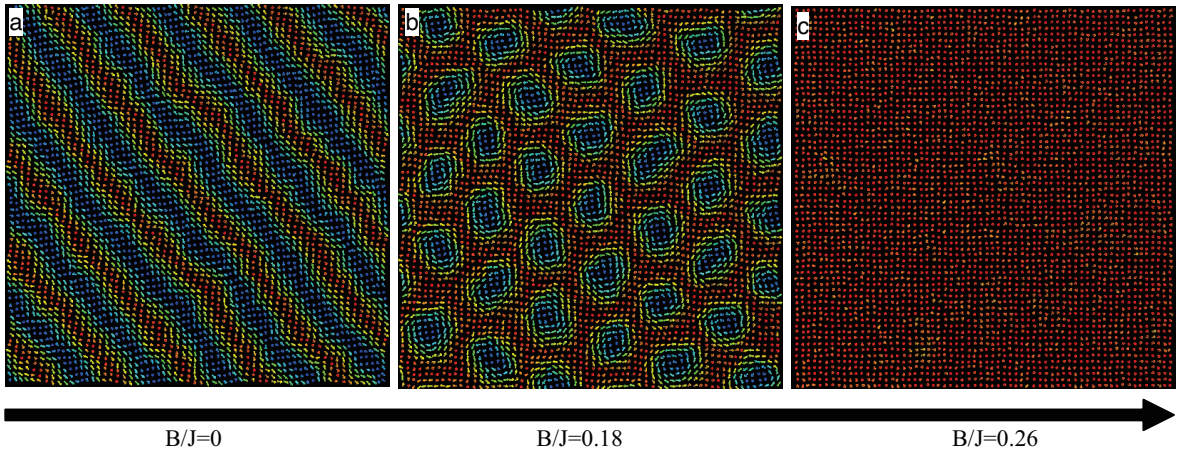


Fig. 6: Phase transition from (a) helical order to (b) Skyrmion crystal and to (c) ferromagnetic order with increasing external magnetic field B/J in 2D squared lattice with 128×128 spins.

As an exmaple, we show in Fig.6 the results of MC simulations for 128×128 spins. As shown in this figure, we have successfully captured the typical phase transitions from helical order to Skyrmion crystal phase and to ferromagnetic order with increasing the magetic field.

Using MC simulation following a simulated annealing techqiue, we have also investigated thew crystalization of magnetic Skyrmion in three spatial dimenstions, and the results are shown in Fig.7. It has been confirmed experimentally that Skyrmions are in cylinder form connecting the top and bottom surfaces of thin film samples. However, the understanding of how the spin changes along the cylinder is still missing. Our simulation can not only reproduce the three-dimensional Skyrmion cylinder consistant with experiments but also uncover the fine-grain spin structures (see Fig. 8). We have found that the Skyrmion is not always perfect especially at the surfaces. On the top (Fig. 8(a)) and bottom surfaces (Fig. 8(c)), we have found that a additional twist exists as compared to the perfect Skyrmion in the middle layer (Fig. 8(b)). We believe that our result would be helpful for experimentist to determine the Skyrmion structure in three spatial dimensions.

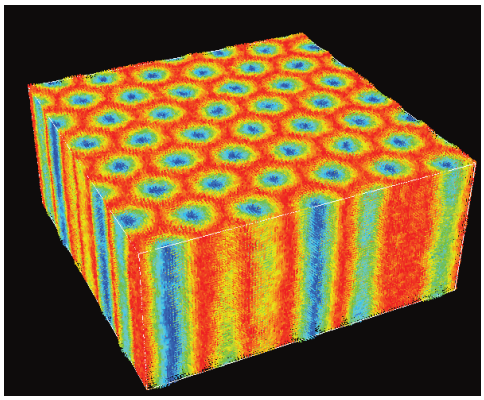
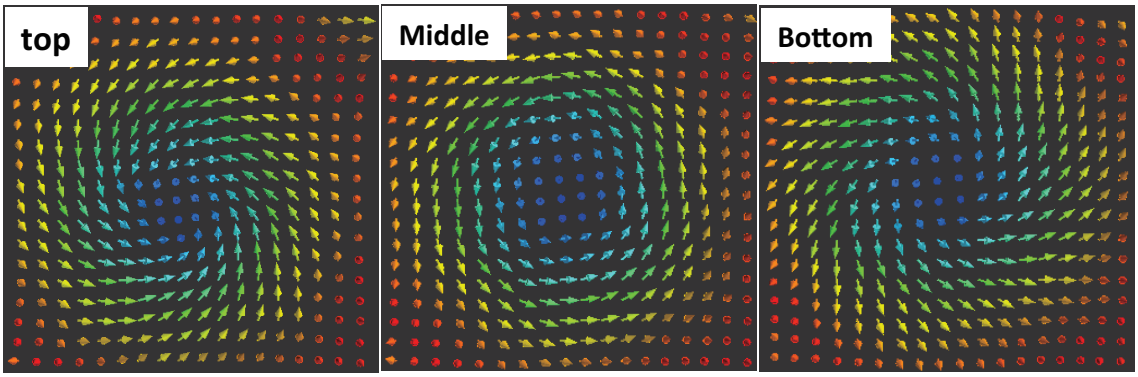


Fig. 7: Spin configurations obtained from MC simulation for 3D cubic lattice with 128×128×58 spins.



(a) (b) (c)

Fig. 8: Spin configuration for a Skyrmion cylinder (shown in Fig.7) on (a) top, (b) middle, and (c) bottom layers.

4. Schedule and Future Plan

4.1 QMC simulations for metal-superconductor transition in interacting Dirac fermions

In the previous study described in 3.1, we have clarified the existence of the universality class in the interacting Dirac fermions, which corresponds to the chiral Heisenberg class in the Gross-Neveu model. Next, we plan to investigate other class of transition in the Dirac fermions, the chiral XY class in the language of the particle physics. We will use the same strategy as before; we will perform the QMC simulations using our highly-improved code for the attractive Hubbard model on lattice systems tuned so that they have the Dirac-like dispersions in the non-interacting limit, where the transition from SM to superconductor occurs at a finite value of the interaction strength. We

expect that this study also leads to the first reliable result for the chiral XY class as in the previous work. Large-scale simulations are essential to address the quantum criticality of the quantum phase transition.

4.2 2D DMRG for strongly correlated quantum systems: dynamical DMRG and time dependent DMRG

We will apply our massively parallelized 2D DMRG algorithm to various strongly correlated quantum systems in both condensed matter physics and quantum chemistry. We will extend our newly developed 2D DMRG algorithm to 2D dynamical DMRG (DDMRG) and 2D time dependent DMRG (tDMRG) methods. Using DDMRG and tDMRG methods, we will investigate real time evolution of cold atoms in optical lattices and spin excitations of spin liquid state in anisotropic Heisenberg model on the triangular lattice, photo-induced phase transitions and the relaxation process. We also plan to extend our 2D DMRG algorithm to a finite temperature 2D DDMRG method.

4.3 MC and MD simulations for chiral magnets

We plan to establish the temperature vs external magnetic filed phase diagram in three dimensions. Experimental observation suggests that the phase diagram strongly depends on the shape of samples. The reason for this is still not completely clear. Numerically, it is also challenging because distinguishing different phases is formidable task. Combining MC and MD methods, we aim to develop an effective code to find stable magnetic structures. We also plan to study dynamics of Skyrmions in three dimensions.

5. Publication, Presentation and Deliverables

(1) Journal Papers

1. “Block Lanczos density-matrix renormalization group method for general Anderson impurity models: Application to magnetic impurity problems in graphene”, T. Shirakawa and S. Yunoki, Phys. Rev B **90**, 195109/1-21 (2014).
2. “Magnetic field effect in one-dimensional charge ordering systems”, Y. Otsuka, H. Seo, and Y. Motome, J. Phys. Soc. Jpn. **84**, 083703/1-4 (2015).
3. “Density-matrix renormalization group study of extended Kitaev-Heisenberg model”, K. Shinjo, S. Sota, and T. Tohyama, Phys. Rev B **91**, 054401/1-10 (2015).
4. “Ultrafast charge and lattice dynamics in one-dimensional Mott insulator of CuO-chain compound Ca2CuO3 investigated by femtosecond absorption spectroscopy”, H. Matsuzaki, H. Nishioka, H. Uemura, A. Sawa, S. Sota, T. Tohyama, and H. Okamoto, Phys. Rev. B **91**, 081114 (R)/1-5 (2015).

5. “0–π transition driven by magnetic proximity effect in a Josephson junction”, S. Hikino and S. Yunoki, J. Phys. Soc. Jpn. **84**, 014712/1-5 (2015).
6. “Giant Switchable Rashba Effect in Oxide Heterostructures”, Z. Zhong, L. Si, Q. Zhang, W.-G. Yin, S. Yunoki, and K. Held, Adv. Mater. Interfaces **2**, 1400445/1-5 (2015).
7. “Spin-orbit-induced exotic insulators in a three-orbital Hubbard model with $(t_{2g})^5$ electrons”, T. Sato, T. Shirakawa, and S. Yunoki, Phys. Rev. B **91**, 125122/1-5 (2015).

(2) Conference Papers

1. “Mott transition in the two-dimensional π-flux phase”, Y. Otsuka, S. Yunoki, and S. Sorella, JPS Conf. Proc. **3**, 013021/1-5 (2014).
2. “Density matrix renormalization group study on a magnetic impurity in the honeycomb lattice”, T. Shirakawa and S. Yunoki, JPS Conf. Proc. **3**, 013025/1-5 (2014).
3. “Temperature dependence of the optical conductivity in a half-filled Hubbard model: Mott-type Insulator vs Slater-type insulator”, K. Seki, T. Shirakawa, and S. Yunoki, JPS Conf. Proc. **3**, 014026/1-6 (2014).
4. “Magnetism in Sr_2IrO_4: a weak coupling study”, K. Nishiguchi, H. Watanabe, and S. Yunoki, JPS Conf. Proc. **3**, 015037/1-6 (2014).
5. “A variational Monte Carlo study of exciton condensation”, H. Watanabe, K. Seki, and S. Yunoki, J. Phys.: Conf. Ser. **592**, 012097/1-7 (2015).
6. “Electronic and magnetic structure under lattice distortion in $SrIrO_3/SrTiO_3$ superlattice: A first-principles study”, W. Fan and S. Yunoki, J. Phys.: Conf. Ser. **592**, 012139/1-6 (2015).

(3) Invited Talks

1. “Superconductivity and metal-insulator transition in Sr_2IrO_4”, S. Yunoki, 2014 EMN Summer Meeting, Cancun, Mexico, June 2014.
2. “Superconductivity and metal-insulator transition in 5d iridium oxides”, S. Yunoki, IUMRS-ICYRAM 2014, Haikou, China, October 2014.
3. “Novel insulator and superconductivity in 5d transition metal iridium oxides in a layered perovskite structyre”, S. Yunoki, 物性研究所計算物性科学センター第 4 回シンポジウム, Chiba, Japan, November 2014.
4. “Application of two-dimensional DMRG method”, S. Sota, Yukawa institute workshop, new trend of study of quantum many particle systems- ― tensor network・renormalization group・entanglement ―, Kyoto, Japan, December 2014.
5. “Large-scale QMC study of Mott transition in interacting Dirac fermions”, Y. Otsuka, S. Yunoki, and S. Sorella, SPring-8 Condensed matter colloquium, Kouto, Japan, January 2015.

6. “The metal-insulator transition for two-dimensional interacting Dirac electrons”, S. Sorella, Y. Otsuka, and S. Yunoki, Advanced Numerical Algorithms for Strongly Correlated Quantum Systems, Würzburg, Germany, February 2015.
7. “Large-scale QMC simulations for Dirac fermions”, Y. Otsuka, S. Yunoki, and S. Sorella, Cyber HPC Symposium, Osaka, Japan, February 2015.
8. “Massively parallel DMRG study on K-computer”, S. Sota, 70th JPS annual meeting, Tokyo, Japan, March 2015.

(4) Posters and presentations

1. “Universal critical behavior of metal-insulator transitions for interacting Dirac fermions”, Y. Otsuka, S. Yunoki, and S. Sorella, JPS 2014 Autumn meeting, Kasugai, Japan, September 2014.
2. “DMRG study of spin frustrated triangular spin model”, S. Sota, K. Shinjo, T. Shirakawa, T. Tohyama, and S. Yunoki, JPS 2014 Autumn meeting, Kasugai, Japan, September 2014.
3. “Massively parallel DMRG method and its application”, S. Sota, CMSI International Workshop 2014: Tensor Network Algorithms in Materials Science, Kobe, Japan, October 2014.
4. “Universal quantum criticality in the 2D interacting Dirac electrons”, Yuichi Otsuka, Seiji Yunoki, and Sandro Sorella, 4th workshop for strongly-correlated electrons, Katsuura Japan, December 2014.
5. “Hydrogen Adsorption on Carbon-Based Materials: Application in Magnetism and Energy Storage”, A. Ranjbar, The 9th General Meeting of ACCMS-VO, Okinawa, Japan, December 2014 .
6. “Dynamical DMRG study of non-linear optical response”, S. Sota and T. Tohyama, 5th CMSI meeting, Sendai, Japan, December 2014.
7. “DMRG study of two-dimensional Hubbard models”, S. Sota, T. Tohyama, T. Shirakawa, and S. Yunoki, International Workshop on New Frontier of Numerical Methods for Many-Body Correlations ― Methodologies and Algorithms for Fermion Many-Body Problems, Tokyo, Japan, February 2015.
8. “Density matrix renormalization group study of triangular Kitaev-Heisenberg model”, S. Sota, K. Shinjo, T. Shirakawa, T. Tohyama and S. Yunoki , APS March Meeting 2015, San Antonio, USA, March 2015.
9. “Two-dimensional DMRG study of two-dimensional Hubbard model”, S. Sota, T. Tohyama, T. Shirakwa, and S. Yunoki, 70th JPS annual meeting, Tokyo, Japan, March 2015.

Computational Biophysics Research Team

1. Team members

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Chigusa Kobayashi (Research Scientist)
Yasuhiro Matsunaga (Research Scientist)
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Tadashi Ando (Research Scientist (Concurrent))*
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Yumi Kashihara (Postdoctoral Researcher (Concurrent))*
Hiromi Kano (Assistant (Concurrent))*
Takaharu Mori (Research Scientist (Concurrent))**
Isseki Yu (Research Scientist (Concurrent))**
Yasuaki Komuro (Student Trainee (Concurrent))**
Raimondas Galvelis (Postdoctoral Researcher (Concurrent))**
Takao Yoda (Visiting Scientist) ***
Mitsunori Ikeguchi (Visiting Scientist)****

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*** The main affiliation is Nagahama Bio Institute.
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2. Research Activities

Molecular dynamics (MD) simulation of biomolecules has become one of the essential research tools in biophysics and biochemistry. The simulation is, in particular, useful for investigating relationships between biomolecular structure and function as well as those between the conformational dynamics and function. One of the major advantages in the simulation is its atomically detailed description of biomolecular structures and dynamics, although the time-scale (< microseconds) is relatively shorter than the typical experimental ones (> milliseconds). Many researchers, therefore, have tried to extend the simulation sizes and lengths by optimization of MD software and/or its algorithms. In our research team, we have developed new high-performance MD software, which we call GENESIS (GENeralized-Ensemble SImulation System) to perform MD simulations of biomolecules efficiently on K computers. At the end of last fiscal year (March, 2014),

we provided the pre-released version of GENESIS as free software under the license of GPLv2 on the team website. In this fiscal year, we developed new algorithms for further optimizations on K computer, sequential data assimilation for combing experimental measurements with simulations, and coarse-grained MD simulations.

3. Research Results and Achievements

3.1 Volumetric decomposition FFT in GENESIS

Many biological applications such as protein folding, aggregation, protein-protein interaction, and so on demand us longr time-scale molecular dynamics (MD) simulations, because these biological phenomena typically occur in the time scale of μsec or msec. For the long time MD simulation, efficient parallelization of MD is essential. However, in the particle-mesh ewald (PME) calculation for long-range electrostatic interaction, the conventional parallelization schemes of fast Fourier transform (FFT) have limited the total performance of MD simulations in massively parallel supercomputers. To overcome the problem, we have developed a new parallelization scheme of FFT. Our method basically makes use of the volumetric decomposition scheme with hybrid parallelization (MPI+OpenMP), which is particularly useful when used in conjunction with the midpoint cell scheme developed in GENESIS. The newly developed parallelization of FFT includes two schemes: 1d_Alltoall with five all-to-all communications in one dimension, and 2d_Alltoall with one two-dimensional all-to-all communications combined with two all-to-all communications in one dimension. Both schemes show comparable or superior performance than existing FFT libraries. The parallel performance on K computer shows the world fastest records of FFT calculations for 512^3 grids and 1024^3 grids, to our best knowledge, improving the performance on large-scale MD simulations greatly. Due to efficient parallelization of FFT, now GENESIS can finish one MD cycle for a virus system containing more than 1 million atoms within 5 ms using 32,768 cores on K computer.

3.2. Development of GENESIS on hybrid CPU+GPUs

The main bottleneck in MD simulations is the calculation of pair-wise non-bonded interactions. Recently, graphics processing units (GPU) become very powerful tools to accelerate the time-consuming real space non-bonded interactions. Nowadays, a lot of MD programs including CHARMM, NAMD, Gromacs, Amber, AceMD, OpenMM, and so on support the use of GPUs. Some of them focus on optimizing on single node without using CPU to remove the data transfer between CPU and GPU. Unlike these programs optimized for single node, we have developed hybrid CPU+GPU calculations on multiple nodes for large-scale MD simulations. First, we introduced new non-bonded interaction scheme suitable for GPU. CPUs have large amounts of cache memory to optimize random memory access. On the other hand, GPUs include very small amount of

cache memory, and instead are optimized for in-order memory access. The global memory size of GPU is usually less than that of CPU. Considering these differences between CPU and GPU, we introduced a new pair-list scheme, which depends on not the pair of atoms but just atom list itself. Although this scheme increases the amount of calculations, computational time could be reduced due to efficient thread calculations on GPU. Moreover, we properly assigned mixed precisions where calculation on GPU is performed using single precision floating points while accumulation is dealt with double precision floating points. Our program is tested on TSUBAME for 1 million atom systems, showing the expected MD simulation time is around 30ns/day using 128 nodes, which is equivalent to the production using 2048 nodes of K computer.

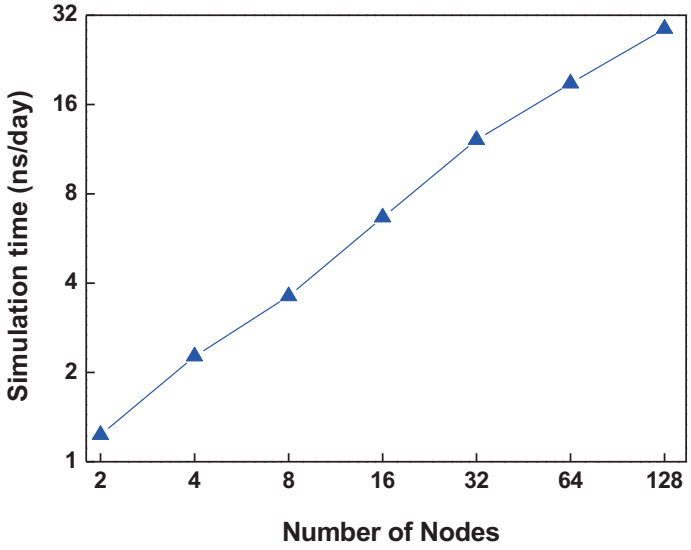

Figure 1. Simulation time versus number of nodes for hybrid CPU+GPU usage of MD simulation.

3.3 Sequential data assimilation for single-molecule FRET data

We have been developing a framework for data assimilation of single-molecule Forster resonance energy transfer (smFRET) data. Data assimilation is a statistical method designed to improve the quality of numerical simulations in combination with real observations. We develop a sequential data assimilation method that incorporates one-dimensional time-series data of smFRET photon-counting into conformational ensembles of biomolecules derived from “replicated" molecular dynamics (MD) simulations. A particle filter using a large number of “replicated" MD simulations with a likelihood function for smFRET photon-counting data is employed to screen the conformational ensembles that match the experimental data. We examined the performance of the method using emulated smFRET data and coarse-grained (CG) MD simulations of a dye-labeled

polyproline-20. The method estimated the dynamics of the end-to-end distance from smFRET data as well as revealing that of latent conformational variables. We also confirmed that the particle filter is also able to correct model parameter dependence in CG MD simulations.

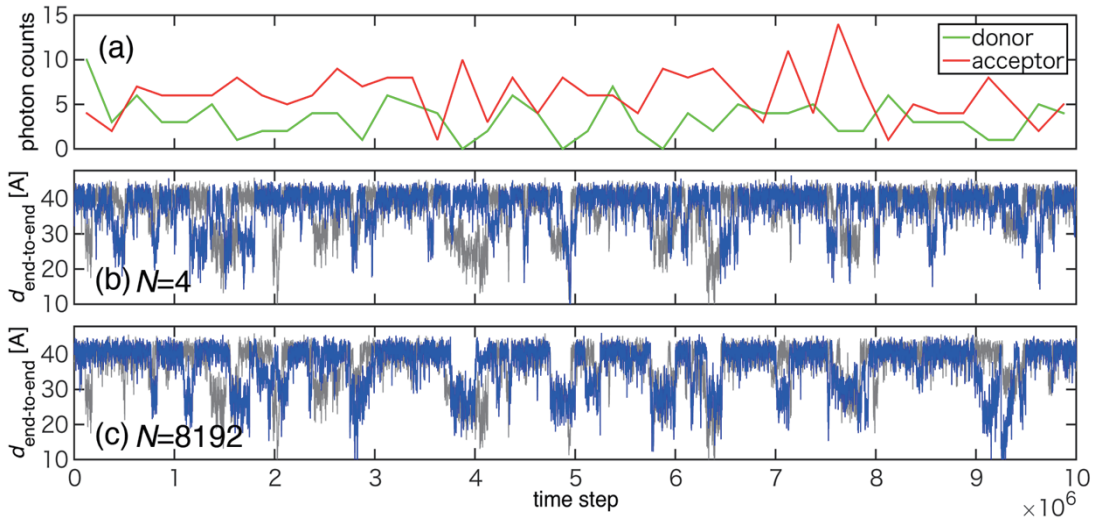

Figure 2. MAP estimates for the end-to-end distance obtained by the particle filter using N=4, and 8192 particles. (a) Emulated smFRET photon-counting data. The photon-counts from the donor and acceptor dyes are indicated by the green and red lines, respectively. (b) The true end-to-end distance obtained in the emulation simulation for smFRET data. (b) MAP estimates by the particle filter using *N*=4 particles is shown with the blue line. The target end-to-end distance (the emulation trajectory data) is indicated with the gray line. (c) MAP estimates by using N=8192 particles.

3.4. Development of coarse-grained MD simulations

Large conformational changes of multi-domain proteins are difficult to be simulated using all-atom models due to the slow time scale of motions. We propose a simple modification in the structure-based coarse-grained (CG) model for stable but efficient MD simulations of those proteins. We first obtain information on the definition of "dynamic domains" and the magnitude of local domain motions in a protein through "Motion Tree", a tree diagram that describes conformational changes in a hierarchical manner from two structures. (Koike *et al.*, *J. Mol. Biol.*, 2014) We recently investigated conformational changes of Ca^{2+}-pump, a multi-domain membrane protein, based on the method and showed that the analysis detects functional motions without extensive biological knowledge of experts. (Journal #2)

In our new CG model, which we call DoME (Domain-Motion Enhanced) model, only the native-contact interaction parameters between two domains are modified as being inversely proportional to the magnitude in "Motion Tree". We applied simulations based on DoME to a small

soluble protein, Adenylate Kinase (AdK), examining the conformational fluctuation in the open state and structural transition between its open and closed states. The simulation results based on DoME are consistent with a 10μsec all-atom MD, previous CGMD simulations, and experimental data. In addition, the simulations based on the model are shown to provide stable trajectories regardless of some temperature differences. We also investigate the conformational transition from the open to closed states in AdK by using a dual-basin Go-model via a perturbation approach proposed by Whitford et al. The comparison suggests that DoME allows us to apply CG MD simulations more easily for multi-domain proteins and provides a stable trajectory that is comparable to experimental studies and long-time all-atom MD simulations.

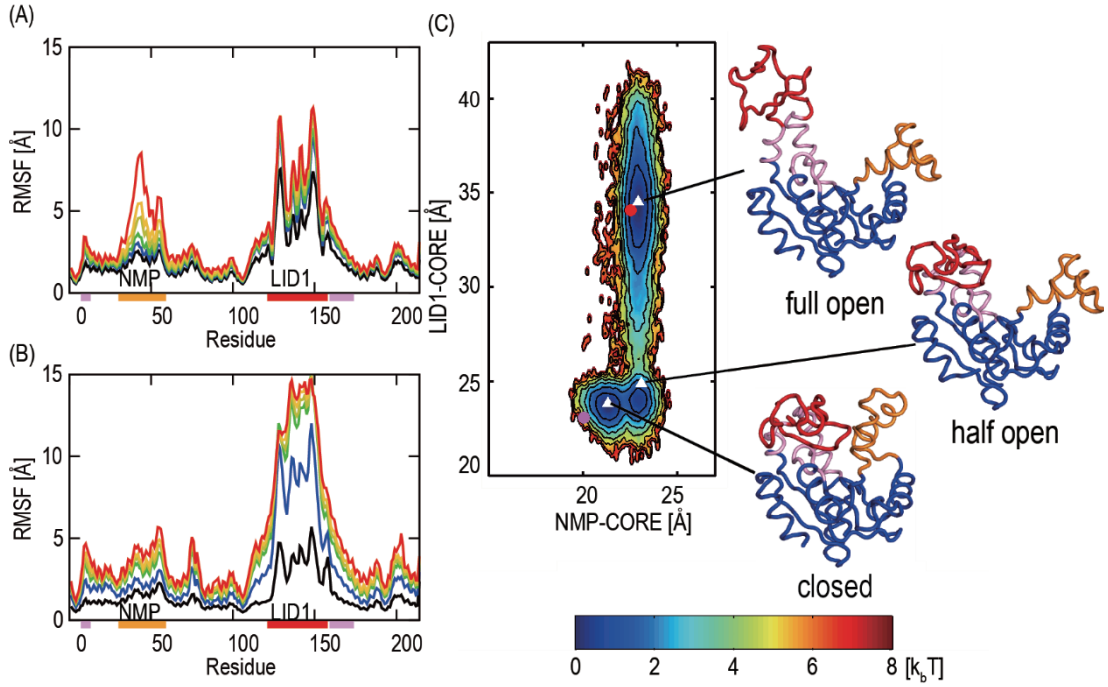

Figure 3. (A-B) RMSFs with different models; (A) the DoME model, (B) the KB (previous) model. Black, blue, green, yellow-green, orange, and red lines are corresponds at different temperatures (C) Free energy surfaces of domain motions with the perturbation DoME model. Vertical and horizontal axes indicate the distance between centers of mass (COMs) of CORE and LID1, and that between COMs of CORE and NMP, respectively. Right side shows structures of three centroids on the free energy surface. (White triangles) Full open, half open, and closed structures are displayed.

3.5. Implementation of new functions in GENESIS

After opening the first version of GENESIS (journal #1), we have implemented the following new functions; 1. GPGPU implementation, (explained in 3.2), 2. Multiple time step integrator (Reversible System Propagator Algorism, RESPA). 3. Enhance available force fields with all atom and CG

models. For efficient sampling with multiple time step integrator, we basically implemented RESPA (Tuckerman *et al, J. Chem. Phys.* 1992) in GENESIS. Long-range interaction described by reciprocal-space interaction is defined as slow motion force and skipped periodically. Based on RESPA, we assigned Langevin thermostat to generate statistically meaningful ensemble spaces. It is revealed that our Langevin RESPA shows better thermodynamic and dynamic properties than the multiple time step integrators using Langevin thermostat and extrapolation. It is also shown that the time step of the slow motion could be increased up to 8 fs with Langevin thermostat while 4-6 fs is the maximum time step with the conventional scheme. In the first version of GENESIS, the standard CHARMM force field files (topology and parameter) are available as input parameters. For coarse-grained model simulations, a Go-model potential developed by Karanicolas and Brooks (Karanicolas and Brooks, *J. Mol. Biol.* 2003) is available. In order to simulate more realistic system, e.g. complex with nucleicacids and glycol-proteins, modules for AMBER and Gromacs force field files have been newly installed. As for CG models, in addition DoME model (explained in 3.4), SMOG (Whitford *et al. Proteins*, 2008) and MARTINI (Marrink *et al . J. Chem. Theo. Comp.*, 2008) models are installed. SMOG and MARTINI models have higher resolution than Karanicolas and Brooks and DoME models. By implementation of different types of CG models, various simulations with multi-scale are available in GENESIS.

4. Schedule and Future Plan

In the next fiscal year, we plan to implement new functions in GENESIS, namely, the reaction path sampling, the flexible collective variables, hybrid QM/MM calculations, and so on. The 2nd version of GENESIS will be released at the end of this fiscal year (March, 2015) also as free software under GPL license v2. For this, we need to test many biological simulations for confirming stable MD simulations using GENESIS.

We will try to simulate slow conformational dynamics of membrane proteins and supramolecules like Ribosome using multi-resolution simulations. So far, we have developed high-performance MD simulations and coarse-grained MD simulations separately. In this fiscal year, we integrate these two simulation modules as well as the reaction path sampling module for this purpose. We will simulate large-scale free-energy calculations of membrane proteins and Ribosomes, using large number of CPUs on K computer.

Hybrid QM/MM calculation is also very important for investigating biological functions of enzymes and proteins. In this fiscal year, new functions including ab initio vibrational analysis and reaction path analysis will be installed in GENESIS in combined with the existing QM programs.

5. Publication, Presentation and Deliverables

(1) Journal Papers

1. Jaewoon Jung, Takaharu Mori, Chigusa Kobayashi, Yasuhiro Matsunaga, Takao Yoda, Michael Feig, and Yuji Sugita, “GENESIS: A hybrid-parallel and multi-scale molecular dynamics simulator with enhanced sampling algorithms for biomolecular and cellular simulations”, WIREs Computational Molecular Science 2015.
2. Chigusa Kobayashi, Ryotaro Koike, Motonori Ota and Yuji Sugita, “Hierarchical domain-motion analysis of conformational changes in sarcoplasmic reticulum Ca^{2+}-ATPase”, Proteins: Structure, Function, and Bioinformatics, 83, pp 746–756, (2015).

(2) Conference Papers

None.

(3) Invited Talks

1. “Molecular mechanism for the drug extrusion by MATE multi-drug transporter”, Yuji Sugita, Functional Computational Changes in Complex Biological Systems, Hong Kong, China, Apr. 2014.
2. “Replica-exchange molecular dynamics simulations for enhanced sampling of biological membrane systems”, Yuji Sugita, Computational Biophysics to Systems Biology (CBSB14), Gdansk, Poland, May. 2014.
3. “Atomistic motions of proteins and water in crowded environments”, Yuji Sugita, Telluride Workshop on Protein and Peptide Interactions in Cellular Environments, Telluride, USA, Jun. 2014.
4. “Domain motion analysis of proteins based on multiple atomic structures and coarse-grained molecular dynamics simulations”, Yuji Sugita, Telluride Workshop on Coarse-grained modeling of structure and dynamics of biomolecules, Telluride, USA, Aug. 2014.
5. “理論・計算化学に基づく脂質ダイナミクスの解析”, Yuji Sugita, 第 87 回日本生化学会大会, Kyoto, Japan, Oct. 2014.
6. “分子動力学計算の高速化と大規模生体分子シミュレーション”, Yuji Sugita, バイオスーパーコンピューティング研究会 2014(第 6 回)総会・講演会, Saitama, Japan, Oct. 2014.
7. 松永康佑 "最小自由エネルギー経路探索法による多剤排出トランスポーターの薬剤排出機構の解明", 第 1 回「京」を中核とする HPCI システム利用研究課題 成果報告会 東京, Oct. 2014.
8. Yasuhiro Matsunaga, “Molecular dynamics simulation studies using multi-copy based methods: string method and sequential data assimilation”, 5th AICS International Symposium, Kobe, Japan, Dec. 2014.

9. “Domain motion analysis of membrane proteins by bioinformatics and molecular dynamics simulations”, Yuji Sugita, The international workshop on computational science and engineering, Hong Kong, China, Dec. 2014.
10. “スーパーコンピュータを用いた細胞内分子ダイナミクスの解析”, Yuji Sugita, ISSP ワークショップ　機能物性融合科学研究会シリーズ(１)「光機能」, Kobe, Japan, Dec. 2014.
11. “Optimization of Molecular Dynamics Program “GENESIS” and its Application to Biomolecular System”, Yuji Sugita, WINTech2015, Kobe, Japan, Mar. 2015.
12. “細胞内分子ダイナミクスのシミュレーションの現状と今後の課題”, Yuji Sugita, よこはま NMR 研究会　第 52 回ワークショップ, Yokohama, Japan, Mar. March 2015.
13. Multiscale molecular dynamics simulations of transmembrane structures of amyloid precursor protein in biological membrane”, Yuji Sugita, 249th ACS National Meeting & Exposition, Denver, USA, Mar. 2015.
14. Jaewoon Jung and Yuji Sugita, “Multiple time step integrator in molecular dynamics (MD) program GENESIS”, IMS2015, Kyoto, March 2015.
15. Yasuhiro Matsunaga, “Drug extrusion mechanism of multidrug transporter AcrB studied by molecular dynamics simulations”, Rare Event Sampling and Related Topics II, The Institute of Statistical Mathematics, Tokyo, Japan, March 2015.

(4) Posters and presentations

1. 小林千草、小池亮太郎、太田元規、杉田有治、 “Conformational changes of SERCA in response to reactions described by hierarchical domain-motion analysis.”, 第 51 回日本生物物理学会年会, 北海道、2014/9/26.
2. 小林千草、小池亮太郎、太田元規、杉田有治、 “Conformational changes of SERCA in response to reactions described by hierarchical domain-motion analysis.”, AICS symposium, Kobe、2014/12/8-12/9.
3. Y. Matsunaga, and Y. Sugita "Sequential data assimilation of single-molecule FRET photon-counting data by using molecular dynamics simulations", Telluride Workshop on Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules, (口頭発表), 2014/8.
4. 松永康佑 "データ同化技術を用いた 1 分子 FRET 計測融合シミュレーションによるタンパク質動態の解明" 第 1 回「京」を中核とする HPCI システム利用研究課題 成果報告会 東京, 2014/10/31.
5. 松永康佑 "1 分子 FRET 光子計数データのモデリング" 新学術領域研究 スパースモデリングの深化と高次元データ駆動科学の創成 2014 年度 公開シンポジウム 東京工業大学, 2014/12/15-17.

6. 松永康佑 "1分子FRET光子計数データのモデリング" 新学術領域研究　スパースモデリングの深化と高次元データ駆動科学の創成 第 2 回領域会議 東京大学, 2014/6/19-21.2

(5) Patents and Deliverables

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)
Yutaka Maruyama (Research Scientist)
Masaki Iwasawa (Postdoctoral Researcher)
Ataru Tanikawa (Postdoctoral Researcher)
Takayuki Muranushi (Postdoctoral Researcher)
Natsuki Hosono (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 an 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.

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).

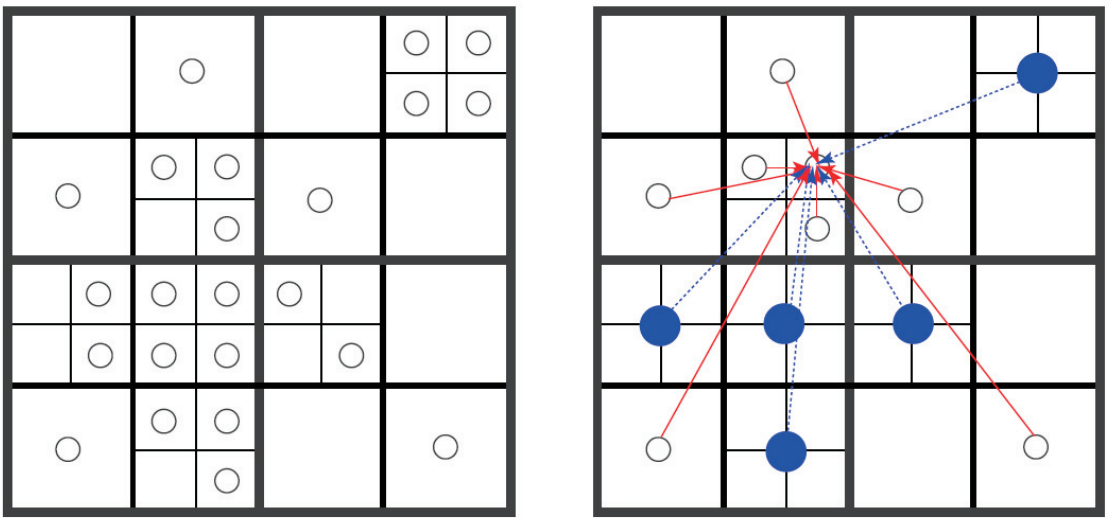

Figure 1. Basic idea of the tree algorithm

The tree algorithm is widely used, but when the periodic boundary condition is applied, we can actually use a more efficient 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.

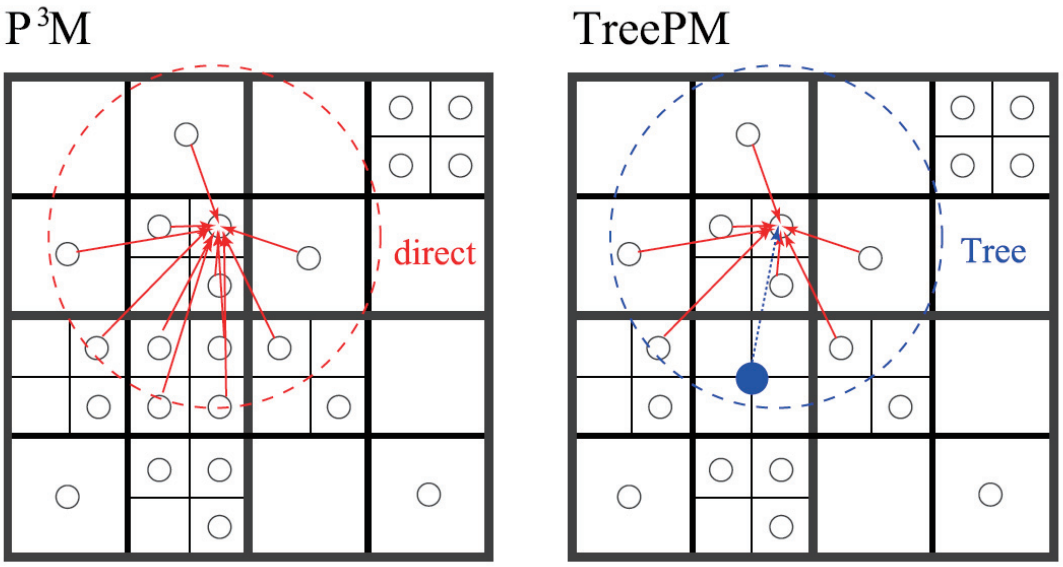

Figure 2. P^{3}M and TreePM

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.

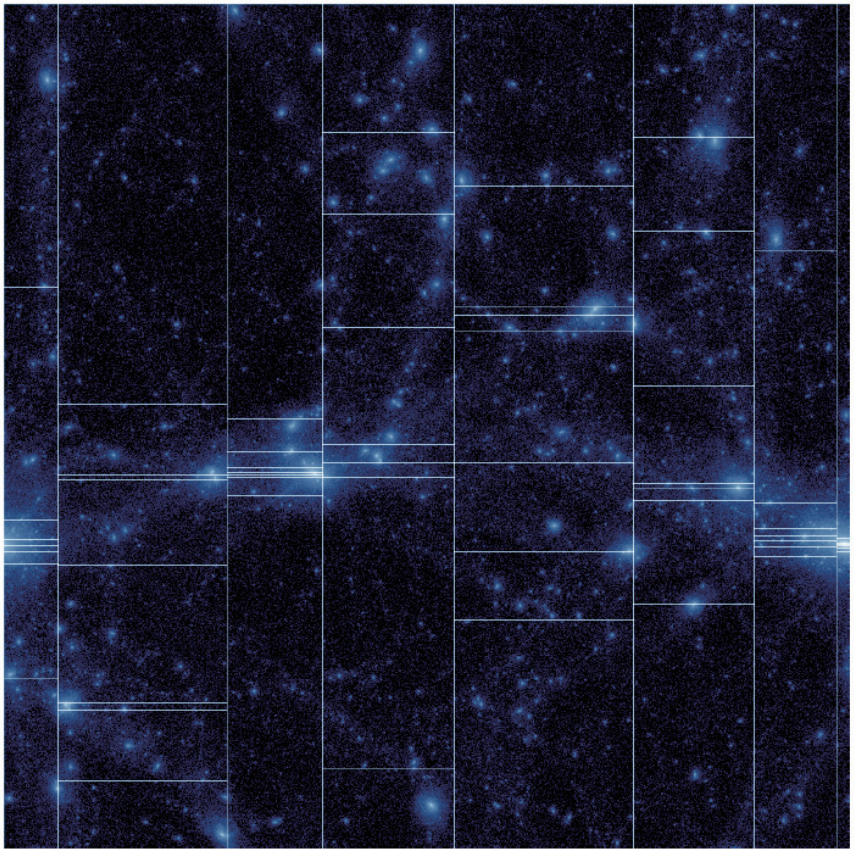

Figure 3 Recursive multisection in two dimension

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 inhomogenous systems.

We used 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 completed and released Version 1.0 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 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 softened 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 multi section 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 multipole 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 successfully implemented all of these functionalities in FDPS version 1.0. (https://github.com/FDPS/FDPS). Using FDPS, a gravitational N-body simulation code can be written in 120 lines, and that code is actually fully scalable even to full-node runs on K computer. For SPH calculations, we have also achieved similar scaling.

FDPS is implemented as a class template library in C++ language. It receives the class definition of particles and a function (or multiple functions in the case of complex interactions) to evaluate the interaction between particles. When a user program is compiled with the FDPS library, the class template is instantiated with the user-specified definition of the particle class. Thus, even though the FDPS library functions are generic ones not specialized to a particular definition of particles, it behaves as if it is a specialized one.

The measured performance of applications developed using FDPS is quite good. Both for gravity-only calculation and SPH calculation, weak-scaling performance is practically perfect, up to the full-node configuration of K computer. Moreover, the measured efficiency, in terms of the fraction of the peak floating-point performance, is also very high. It is around *50%* for gravity-only calculation. For SPH calculations, at the time of writing the performance is around *10%*.

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. The reason is that the formulation of the standard SPH requires that the density is differentiable, which is by definition no the case at the contact discontinuity.

We have been working on the possible solution on this problem. One approach is to reformulate SPH so that it does not use the density in the right-hand side of the equation of motion. We one way to achieve the density independence. 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.

We are also working on a completely different approach, in which we replace the SPH formulation to evaluate the gradient to other schemes. SPH has a known problem that its kernel estimate contains O(1) error, since the summation of contributions from neighbor particles is not guaranteed to be unity. The reason why SPH uses this mathematically inconsistent formulation is to achieve symmetry and conservation. In SPH discretization, interaction between two particles is symmetric, which guarantees the conservation of linear and angular momenta. However, the use of SPH

approximation resulted in rather low accuracy, which limits the reliability of the results obtained using SPH. We are experimenting with several different schemes which can achieve much higher accuracy, while losing some of the nice features of SPH such as the symmetry of interaction.

4. Schedule and Future Plan

We plan to improve the performance of FDPS further in FY 2015. In particular, we plan to extend the API so that the users of FDPS can easily use heterogeneous machines such as machines with GPGPUs or Intel MIC.

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. "Binary formation in planetesimal disks. II. Planetesimals with a mass spectrum". Kominami, J. D., Makino, J. , Publications of the Astronomical Society of Japan 66, 123. 2014
2. "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 440, 652-662. 2014

(2) Conference Papers

1. "Nanoblock Unroll: Towards the Automatic Generation of Stencil Codes with the Optimal Performance", Takayuki Muranushi; Keigo Nitadori, Junichiro Makino, Proceedings of the Second Workshop on Optimizing Stencil Computations, 49-55
2. "Systems Demonstration: Writing NetBSD Sound Drivers in Haskell", Takayuki Muranushi; Motomu Okabe, 2014 ACM SIGPLAN Symposium on Haskell, 77-78
3. "Experience Report: Type-checking Polymorphic Units for Astrophysics Research in Haskell", Takayuki Muranushi; Richard A. Eisenberg, 2014 ACM SIGPLAN Symposium on Haskell, 31-38
4. "24.77 Pflops on a gravitational tree-code to simulate the Milky Way Galaxy with 18600 GPUs", Jeroen Bédorf, Evghenii Gaburov, Michiko S. Fujii, Keigo Nitadori, Tomoaki Ishiyama, and Simon Portegies Zwart, In Proceedings of the International Conference for

High Performance Computing, Networking, Storage and Analysis (SC '14), 54-65

(3) Invited Talks

1. 谷川　衝「銀河中における巨大ブラックホールの合体と成長の研究」、谷川衝、「超巨大ブラックホール研究推進連絡会」第２回ワークショップ、2014/11/3-4、筑波大学
2. 谷川　衝「中間質量ブラックホール」、第１３回 DECIGO ワークショップ、2014/10/26、京都大学
3. 谷川　衝「星団の力学進化と恒星進化」、第１回 DTA シンポジウム「星形成領域および星団環境での惑星の形成と進化」、2014/9/29-30、国立天文台
4. Keigo Nitadori “A block-step version of KS regularization”, Steller N-body Dynamics, 2014/9/10, Sexten Center for Astrophysics,Italy
5. 牧野　淳一郎　エクサスケールコンピュータとその上での分子シミュレーション 第 28 回分子シミュレーション討論会 2014/11/13 仙台
6. 牧野　淳一郎　ゴードン・ベル賞ってどんなもの？ --- 歴史と意義 理研東京事務所記者勉強会 2014/11/11
7. 牧野　淳一郎　スーパーコンピューターの歴史 --- 「京」コンピュータまで、その先 PDF 北大での講義 1 コマ 2014/10/30
8. 牧野　淳一郎　HPC と省電力設計 Calypto Uses Forum 2014 2014/08/29
9. 粒子法の大規模並列化フレームワークと SPH 法に関するいくつかの話題先駆的科学計算に関するフォーラム 20142014/08/5-6

(4) Posters and presentations

1. 細野　七月　“iSALE と粒子法コードの比較に向けて”、2014/10/11、日本惑星科学会
2. 細野 七月　“Terrestrial magma ocean origin of the moon”、2014/10/23-25、衝突研究会
3. 谷川　衝「連星白色矮星の合体と Ia 型超新星」、第 27 回 理論懇シンポジウム 「理論天文学・宇宙物理学と境界領域」、2014/12/24-26、国立天文台
4. 谷川　衝「連星白色矮星の合体と Ia 型超新星」、第２回 DTA シンポジウム「コンパクト天体の活動性と磁気的性質」、2014/10/27-29、国立天文台
5. 谷川　衝「連星白色矮星の合体に伴う星周物質の形成」、日本天文学会２０１４年秋季年会、2014/9/11-13、山形大学
6. 岩澤全規　“Particle-Particle Particle-Tree(P3T)法の GPU への実装及び高密度星団系への応用”、2014/9/11、日本天文学会 2014 年秋季年会
7. anikawa, A. “Detection rate of binary black holes formed in globular clusters”, 3-7 Jun 2013, Yukawa Institute for Theoretical Physics Kyoto University, Yukawa International Seminar 2013 Gravitational Waves Revolution in Astronomy & Astrophysics

(5) Patents and Deliverables

1. FDPS https://github.com/FDPS/FDPS

(6) Awards

Computational Climate Science Research Team

1. Team members

Hirofumi Tomita (Team Leader)
Yoshiyuki Kajikawa (Senior Scientist)
Shin-ichi Iga (Research Scientist)
Seiya Nishizawa (Research Scientist)
Hisashi Yashiro (Research Scientist)
Sachiho Adachi (Research Scientist)
Yoshiaki Miyamoto (Special Postdoctoral Researcher)
Yousuke Sato (Postdoctoral Researcher)
Tsuyoshi Yamaura (Postdoctoral Researcher)
Ryuji Yoshida (Postdoctoral Researcher)
Hiroaki Miura (Visiting Researcher)
Mizuo Kajino (Visiting Researcher)
Hiroshi Taniguchi (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 have aimed to construct a new climate model based on the further theoretically physical principles. Conducting such a new 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 another numerical technique should be needed under the collaboration of hardware research and software engineering for the effective use on the future HPC, including the K computer and Post 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 build a next-generation climate model. The establishment of the above basic and infrastructure research on the K Computer is strongly required, because this research leads to the post K computer or subsequent ones in the future.

We continue to conduct four ongoing projects in this fiscal year as following.

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). We develop a new library for numerical simulation. The progress in development of SCALE, SCALE-LES and NICAM is reported.
2. Simulation of the transition from closed cell to open cell off the west coast of California:
   In order to achieve an outstanding simulation of SCALE-LES on the K computer, our team conducted the simulation with the high resolution and longer integration to demonstrate the shallow clouds.
3. Grand challenge run for sub-km horizontal resolution run by global cloud-resolving model:
   Another outstanding simulation of global model NICAM on the K computer, with super-high resolution (870m), has been done. We analyze the simulation in cooperation with the SPIRE3. We report the analysis of convection properties in the simulation.
4. 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 for.

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 for developing new ones which are suite on massive parallel computers especially the 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 the K computer and is available for the K computer users as an AICS Software (http://www.aics.riken.jp/en/kcomputer/aics-software.html). In this year, we developed components which are necessary for real atmospheric simulations; a boundary turbulence scheme, an urban canopy model, nesting system, and preprocessing tools. We also have improved the library and the model for better performance in both physical and computational aspects.

Development of global atmosphere model NICAM:

Nonhydrostatic ICosahedral Atmosphere Model (NICAM) is used in many of research project on the K computer; for example, HPCI SPIRE field 3, HPCI General Use program (e.g. hp140046: global pollution simulation), and collaborative research with Data Assimilation Research Team in AICS. Productive NICAM simulations show high performance (7-10% of peak) and good scalability (from 10nodes to 20480nodes). Responding the increase of use scene, we developed new components of NICAM. Further improvement of the computational performance on the K computer was also conducted.

Improvement of the stencil operation core: NICAM adopts finite-volume method and horizontal explicit and vertical implicit (HEVI) scheme to solve the Navier-Stokes equations. The part of the geophysical fluid dynamics solver in NICAM is extracted as “Dynamical Core” and packaged to NICAM-DC. We have enhanced the test case of global fluid dynamics following the “Dynamical Core Model Intercomparison Project (DCMIP)”.

Development of the river components: For the ocean-atmosphere coupling simulation, coupling library have been developed in the JST CREST program (Development of System Software Technologies for post-Peta Scale High Performance Computing). In collaboration with this program, we implemented the river component of NICAM. The river is important to balance the incoming water from atmosphere via land to the ocean and outgoing (evaporating) water from ocean to the atmosphere. The river submodel is based on the TRIP model (Oki and Sud, 1998). The distances between source and destination point of flow-down are not always 1 grid (neighbor) but 2-4 grids. On the multi-node (MPI) parallel execution, the river-flow needs network communication, which is different from halo exchange for stencil calculation. We have newly developed communication kernel for the general point-to-point data movement on the NICAM’s massively parallel framework with icosahedral grid system. Figure 1 shows the sample result of global river storage. The river flow from continent to the ocean is visualized (e.g. Nile river and Amazon River).

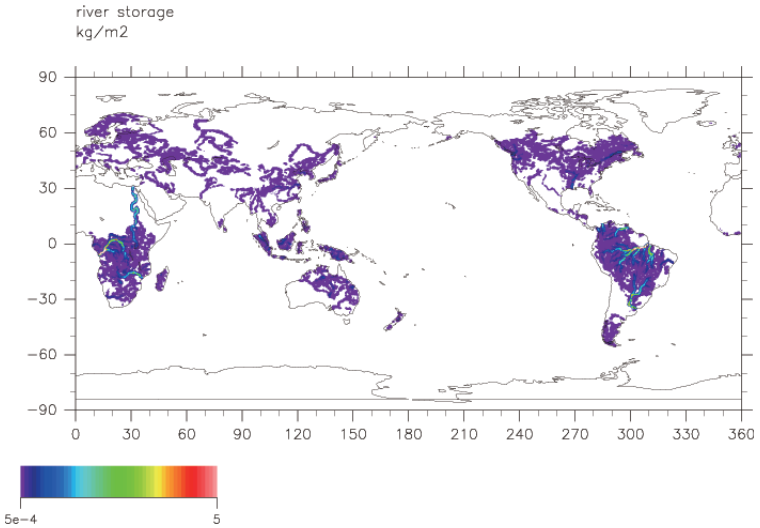

Figure 1: A sample of global distribution of river storage [kg/m2], calculated by the NICAM

Development of the ocean components: Atmosphere faces

the ocean water at the bottom boundary. NICAM uses “slab” ocean component in default. The slab ocean submodel provides ocean surface condition such as sea surface temperature and sea ice amount, with responding the energy/water inflow/outflow of the atmosphere. The water depth of the mixing layer near the sea surface is an important parameter of slab ocean, which affects to the temporal and spatial variation of atmosphere-ocean heat exchange. We implemented a new sub-grid model in mixing layer of slab ocean submodel. The model is based on the Kawai and Wada (2007). The depth of mixing layer is diagnosed from accumulated, net energy input (wind stress, heat exchange, precipitation, evaporation and solar radiation) to the lowermost layer of the ocean. Figure 2 shows the global distribution of mixing layer depth, simulated by using new ocean sub-layer component. The difference of the depth between tropical region and mid- and high- latitude region is reproduced more realistically.

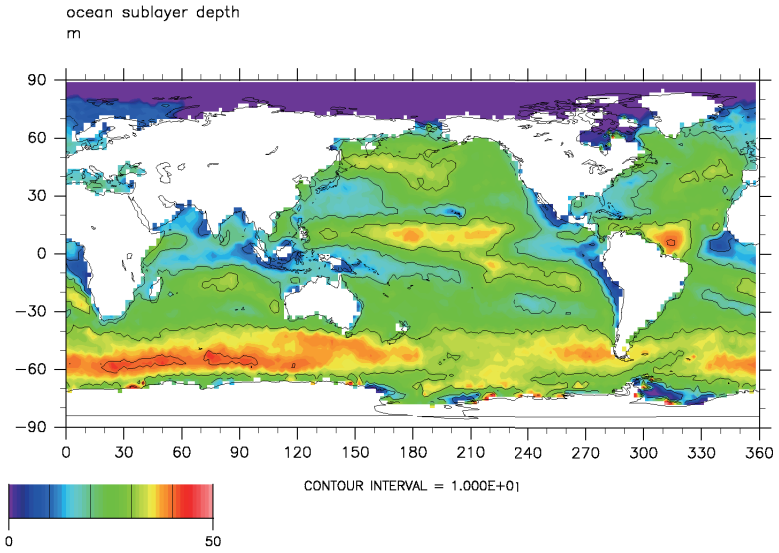

Figure 2: A sample of global distribution of mixed layer depth [m] calculated by the NICAM

3.2 Simulation of the transition from closed cell to open cell off the west coast of California

Using SCALE-LES model, we have investigated shallow clouds (e.g. stratus, stratocumulus, cumulus), which have important role in energy budget of the Earth through radiative process. The cloud cover largely contributes to determine the radiative properties of shallow clouds. Thus, the transition from low cloud cover to high cloud cover is one of the important processes. To investigate the key mechanism determining the cloud cover, we conducted the numerical simulation of the transition in a single calculation domain covering extremely wide calculation domain (300 × 28 × 1.7 km^3) with extremely fine grid resolution (dx = dy = 50m, dz = 5m). The transition from high cloud cover (“cumulus under stratocumulus”) to low cloud cover (“isolated cumulus”) was reproduced successfully as shown in Figure 3. Through the analysis of the results, we proposed a concept to explain how the cloud cover is determined; the relationship between “cloud broadening

distance" and "distance of each cumulus" determines cloud cover.

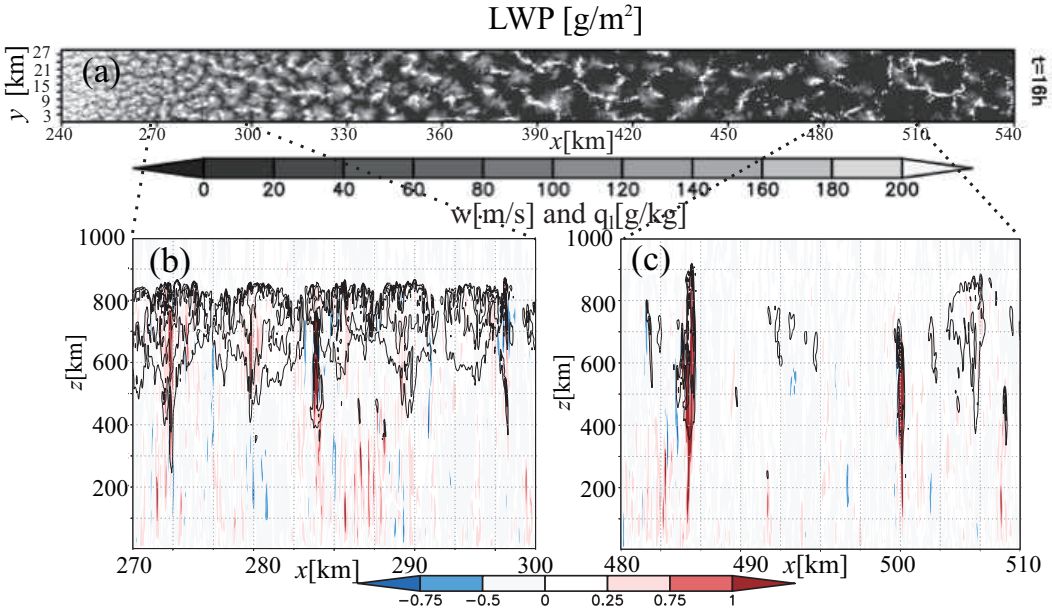

Figure 3: Spatial distribution of (a) the liquid water path at t = 16 h. The x–z slice shows the liquid water mixing ratio (ql = qc+qr) (contour) and vertical velocity (shaded) at t = 16 h in (b) 270km < x < 300 km, y = 15 km and (c) 480 km < x < 510 km, y = 15 km. The contour line in (b) and (c) corresponds to 0.25, 0.5, 0.75, and 1.0 g kg-1, respectively.

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

Analysis of global sub-km experiment

Using the K computer, we have succeeded in conducting the global simulation with the world's highest resolution, 870 m. The result of analyses of deep atmospheric convection using the simulation data has been published in 2013 (Miyamoto et al. 2013). We showed that the convection that plays a key role in global atmospheric motion is resolved when the resolution is less than 2-3 km.

We started additional analyses to reveal the differences in convection properties in various atmospheric disturbances. Various cloudy disturbances always exist in the Earth's atmosphere, and they play important roles in global energy budget. Since their element is the convection, we focused on the differences in convection under four representative cloudy disturbances: Madden-Julian Oscillation (MJO), Tropical Cyclones (TC), Mid-latitudinal Lows (MDL), and Fronts (FRT). The paper describing the results was published in the 2014 fiscal year (Miyamoto et al. 2015). We first defined the four disturbances and then detected the convection from the subkilometer simulation.

Taking composites of convective properties such as vertical velocity (w) and precipitation revealed that the convection structures are significantly different (Fig. 4). In the tropical disturbances, MJO and TC, the convection is tall consistent with the tropopause height. On the other hand, the midlatitudinal disturbances, MDL and FRT, have short convection. The MJO convection is strongest out of the four and it is stronger than the global average. In contrast, the TC convection is relatively weak. It may be interpreted by the environmental factors of convection in the two disturbances. In MJO (TC), convective available potential energy is large (weak), whereas low-level convergence is weak (strong). Thus, the convection in MJO can obtain more energy than TC. The convection in TC appears to be forced to form by the strong convergence caused by the TC vortex. The difference between MDL and FRT can be interpreted in the similar way.

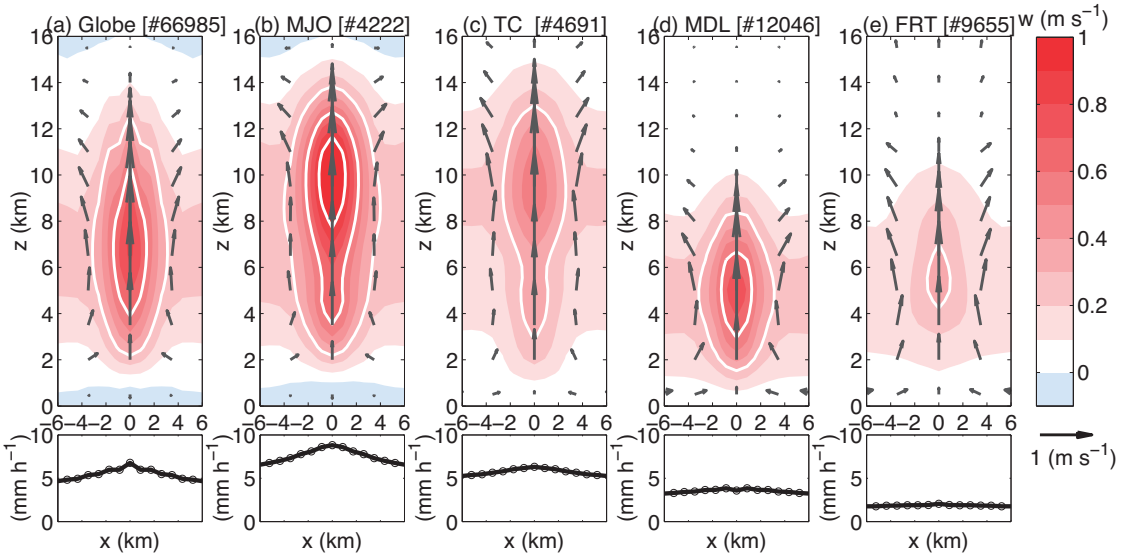

Figure 4: (Top) Radius-height composites of vertical velocity (w, shaded) and velocity vector of radial and vertical velocities (arrows) for the simulated convection detected in (a) the globe, (b) MJO, (c) TC, (d) MDL, and (e) FRT. The white contours of w are at w = 0.3, 0.6 and 0.9 m s-1. The number of convection cells is shown in the figure title. (Bottom) Radial distributions of composited precipitation. (Figure 2 of Miyamoto et al. 2015)

3.4 Hyogo-Kobe COE establish project

We conducted four months timeslice experiment using SCALE-LES with the boundary data of NICAM AMIP-type experiment, to validate the model performance on the climate simulation around the Hyogo/Kobe area. The simulation period of each timeslice run was five days including first-one day for the spinup. The horizontal grid interval of the model was 7.5km, 2.5km, and 0.5km for the domains 1, 2, and 3, respectively. The output from the innermost domain (domain 3) was

used for analysis.

The amount and spatial distribution of four-month mean precipitation were successfully simulated by SCALE-LES and agreed well with the observation, although the simulated precipitation was overestimated in the mountain areas. In addition to the spatial distribution, the occurrence frequency of hourly precipitation in the Kansai region was also successfully represented by SCALE-LES, as shown in Fig. 5. The frequency of heavy rainfall more than 50 (mm/hr) is different between the observation and model result. This is because the number of heavy rainfall event varies depending on the year, namely, one year for the simulation is not enough for the climatological analysis of heavy rainfall. From these analyses, we validated the utility of SCALE-LES for the climate simulation around the Hyogo/Kobe area. On the other hand, several issues become identified such as the model biases described above. After the improvement of the model performance, we will start the long-term climate simulation in the next fiscal year.

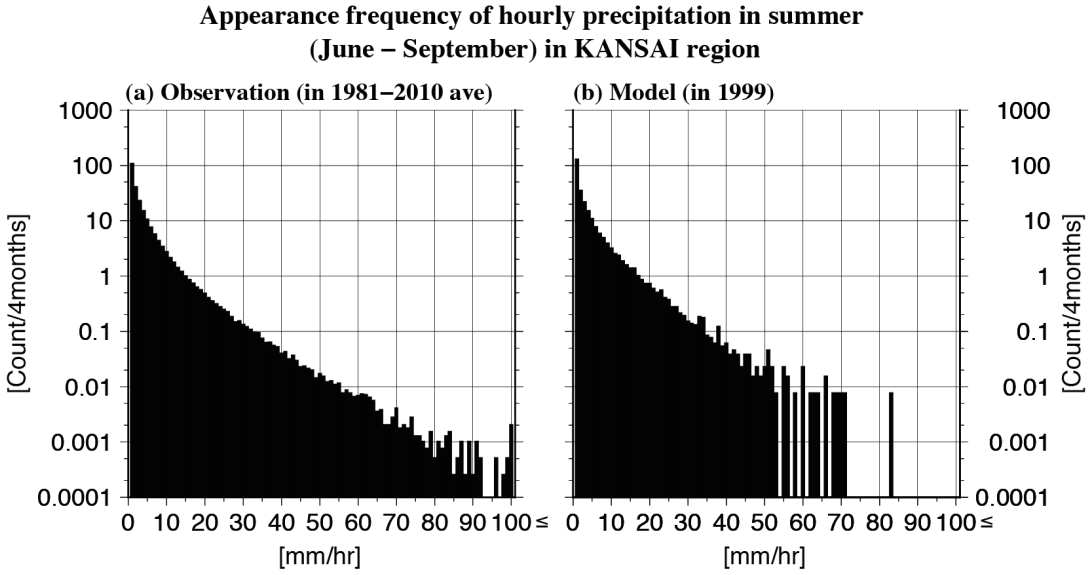

Figure 5: Appearance frequency of hourly precipitation from June to September in the Kansai region: (a) AMeDAS observation averaged between 1981 and 2010, (b) simulation by SCALE-LES averaged in 1999.

5. Schedule and Future Plan

In the next year, we will continue to develop, update and maintain the numerical library for the K computer (SCALE library). Cumulus parameterization and high-accuracy dynamical scheme will be implemented. We also try to enhance the performance of each existing scheme. At the same time, we will work on the following three projects in the collaboration with other team in AICS and the scientist in other institute.

(1) On the Hyogo/Kobe COE establish project, we will conduct the long-term climate simulation by using SCALE-LES to examine the heavy rainfall over Kobe city area. NICAM AMIP-type run for the current climate will be used for the boundary. We will obtain the geographical distribution of the frequency of heavy rainfall and evaluate it with the observational datasets provided by Kobe/Hyogo government. We will also conduct the future climate simulation and highlight the future change of the local heavy rainfall.

(2) 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. In collaboration with the Data Assimilation team in AICS, we contribute to develop the SCALE-LETKF (Local Ensemble Transform Kalman Filter).

(3) We join the POST K Science priority project under the collaboration with JAMSTEC. NICAM-LETKF is one of the target applications. Our team will continue to develop and update that application.

The comprehensive analysis of the two grand challenges run by NICAM and SCALE-LES before will be wrapped up. The new concept for the profitability of deep convection will be established and highlighted by using NICAM simulation results. Comprehensive understanding of the Shallow clouds will be advanced with the result of SCALE-LES.

5. Publication, Presentation and Deliverables

(1) Journal Papers

1. Kodama C., M. Terai, A. T. Noda, Y. Yamada, M. Satoh, T. Seiki, S. Iga, H. Yashiro, H. Tomita, and K. Minami, 2014 : Scalable Rank- Mapping Algorithm for an Icosahedral Grid System on the Massive Parallel Computer with a 3-D Torus Network, Parallel Computing, 40, 8, 362-373, doi:10.1016/j.parco.2014.06.002.
2. Kodama C., S. Iga, and M. Satoh, 2014: Impact of the Sea Surface Temperature Rise on Storm-Track Clouds in Global Non-hydrostatic Aqua-Planet Simulations, Geophys. Res. Lett., 41, 10, 3545-3552, doi:10.1002/2014GL059972.
3. Y Tsushima, S. Iga, H. Tomita, M. Satoh, A. T. Noda, and M. J. Webb, 2014: High cloud increase in a perturbed SST experiment with a global nonhydrostatic model including

explicit convective processes, Journal of Advances in Modeling Earth Systems, 6, 3, 571–585, doi:10.1002/2013MS000301.

4. Satoh M., H. Tomita, H. Yashiro, H. Miura, C. Kodama, T. Seiki, A. T Noda, Y. Yamada, D. Goto, M. Sawada, T. Miyoshi, Y. Niwa, M. Hara, T. Ohno, S. Iga, T. Arakawa, T. Inoue, and H. Kubokawa, 2014: The non-hydrostatic icosahedral atmospheric model: description and development, Progress in Earth and Planetary Science, Progress in Earth and Planetary Science, 1, 18, doi:10.1186/s40645-014-0018-1.
5. Yamaura T., and T. Tomita, 2014: Two Physical Mechanisms Controlling the Interannual Variability of Baiu Precipitation , Journal of the Meteorological Society of Japan, 92, 4, 305-325, doi:10.2151/jmsj.2014-403.
6. Yun K.-S., K.-J. Ha, J.-Y. Lee, and Y. Kajikawa, 2014: Interdecadal Changes in the Asian Winter Monsoon Variability and Its Relationship with ENSO and AO, Asia-Pac. J. Atmos. Sci., 50, 4, 1-10, doi:10.1007/s13143-014-0042-5.
7. Miyakawa T., M. Satoh, H. Miura, H. Tomita, H. Yashiro, A. T. Noda, Y. Yamada, C. Kodama, M. Kimoto and K. Yoneyama, 2014: Madden–Julian Oscillation prediction skill of a new-generation global model demonstrated using a supercomputer, Nature Communications, 5, 3769. doi:10.1038/ncomms4769.
8. Miyamoto Y., R. Yoshida, T. Yamaura, H. Yashiro, H. Tomita and Y. Kajikawa, 2014: Does convection vary in different cloudy disturbances?, Atmos. Sci. Lett., accepted.
9. Tsushima Y., S. Iga, H. Tomita, M. Satoh, A. T. Noda, and M. Webb, 2014: High cloud increase in a perturbed SST experiment with a global nonhydrostatic model including explicit convective processes, Journal of Advances in Modeling Earth Systems, 06, 571-585, doi:10.1002/2013MS000301.
10. Seiki T., M. Satoh, H. Tomita, and T. Nakajima, 2014: Simultaneous evaluation of ice cloud microphysics and non-sphericity of the cloud optical properties using hydrometeor video sonde and radiometer sonde in-situ observations, J. Geophys. Res. Atmos., 119, 6681-6701, doi:10.1002/2013JD021086.
11. Yashiro H., A. Naruse, R. Yoshida, and H. Tomita, 2014: A Global Atmosphere Simulation on a GPU Supercomputer using OpenACC: Dry Dynamical Core Tests, TSUBAME e-Science Journal (ESJ), 12, 8-12,
12. 宮本佳明, 2014: Maximum Potential Intensity (新用語解説), 天気, 61(9), 799-801, http://www.metsoc.jp/tenki/pdf/2014/2014_09_0043.pdf.
13. 八代尚, 富田浩文, 宮本佳明, 2014: スーパーコンピュータ「京」の利用：5. 1km 格子間隔を切る大気大循環シミュレーションへの道のり, 情報処理学会誌「情報処理」55, 8, 811-816, http://id.nii.ac.jp/1001/00102187/.

(2) Invited Talks

14. Yashiro H., Recent performance of NICAM on the K-computer and activities towards post-petascale computing, Workshop on Scalability, Reading, United Kingdom, April 14-15, 2014.(Invited)
15. Tomita H., Numerical techniques of cloud resolving model and large eddy simulation on the future HPC system, World Weather Open Science Conference 2014, Montreal, Canada, August 16-21, 2014.(Invited)
16. Tomita H., A numerical technique of global CRM and LES on future high performance computer, 2014 KIAPS International Symposium, Seoul, Korea, October 27-29, 2014.(Invited)
17. Yashiro H., M. Satoh, and H. Tomita, NICAM 870m mesh simulations on the K computer and a road toward global LES, AGU fall meeting, San Francisco, CA, USA, December 15-19, 2014.(Invited)
18. Tomita H., Climate Projection and Numerical Weather Prediction toward the Exa-Scale Era, International Super Computing Conference, Leipzig, Germany, June 22–26, 2014.(Invited)
19. Tomita H., Requirement of simulation code for big data assimilation, The fourth International Symposium on Data Assimilation, Kobe, Japan, February 23-27, 2015.(Invited)
20. Yashiro H., A Simulation of Global Atmosphere Model NICAM on TSUBAME2.5 Using OpenACC, GPU Technology Conference 2015, San Jose, CA, USA, March 16-20, 2015.(Invited)
21. 富田浩文, 京を使った高解像度全球大気シミュレーションの成果とこれからの展望, SS 研 HPC フォーラム 2014 Bridge to Exa ～アプリケーションの観点から～, 東京(汐留シティセンター), Aug 26, 2014.(Invited)

(3) Posters and Presentations

22. Miyamoto Y., T. Takemi, A Triggering Mechanism for the spontaneous axisymmetric intensification of tropical cyclones, 31st Conference on Hurricanes and Tropical Meteorology, San Diego, CA, USA, March 31-April 4, 2014.(Oral)
23. S. Iga, H. Tomita, Improved Smoothness and homogeneity of icosahedral grids using the spring dynamics method, PDEs 2014 Science Workshop, Boulder, CO, USA, April 7-11, 2014.(Oral)
24. Kajikawa Y.,T. Yamaura, H. Tomita, M. Satoh, Indian Summer Monsoon Onset in 2012 Simulated by Global Cloud-system Resolving Model NICAM, Takio Murakami Memorial Symposium on Tropical Meteorology and Monsoon, Honolulu, HI, USA, July 2-3, 2014.(Oral)

25. Sato Y., S. Nishizawa, H. Yashiro, Y. Miyamoto, H. Tomita , Transition from closed cell to open cell structure of stratocumulus simulated by high resolution Large Eddy simulation model covering wide calculation domain, 14th Conference on Cloud Physics, Boston, MA, USA, July 7-11, 2014.(Poster)
26. Nishizawa S., H. Yashiro, M. Odaka, Y. Takahashi, Y. Hayashi, H. Tomita, S. Takehiro, M. Ishiwatari, K. Nakajima, Y. Sato, K. Sugiyama, High-resolution Large-eddy Simulation of the Martian Planetary Boundary Layer, AOGS 11th Annual Meeting, Sapporo, Japan, July 28-August 1, 2014.(Poster)
27. Sato Y., S. Nishizawa, H. Yashiro, Y. Miyamoto, H. Tomita, Potential of Retrieving Shallow-cloud Life Cycle from Next Generation Satellite Observations Through Cloud Evolution Diagrams: a Suggestion from a Large Eddy Simulation, AOGS 11th Annual Meeting, Sapporo, Japan, Jul 28y-August 1, 2014.(Poster)
28. Kajikawa Y., T. Yamaura, H. Tomita, M. Satoh, Indian Summer Monsoon Onset in 2012 Simulated by Global Cloud-system Resolving Model NICAM, AOGS 11th Annual Meeting, Sapporo, Japan, July 28-August 1, 2014.(Poster)
29. Yoshida R., Y. Kajikawa, H. Ishikawa , Impact of Boreal Summer Intraseasonal Oscillation on Environment of Tropical Cyclogenesis Over the Western North Pacific, AOGS 11th Annual Meeting, Sapporo, Japan, July 28-August 1, 2014.(Poster)
30. Yashiro H., Y. Kajikawa, Y. Miyamoto, R. Yoshida, T. Yamaura, H. Tomita, Diurnal Cycle of the Precipitation in a Sub-kilometer Global Simulation, AOGS 11th Annual Meeting, Sapporo, Japan, July 28-August 1, 2014.(Poster)
31. Kajikawa Y., Y.-W. Seo, K.-S. Yun, K.-J. Ha, R. Johnson, Role of the SST Over the East China Sea in the Linkage Between East Asian Winter and Summer Monsoon Variability, AOGS 11th Annual Meeting, Sapporo, Japan, July 28-August 1, 2014.(Oral)
32. Yamaura T., T. Tomita, Two Physical Mechanisms in the Interannual Variability of Baiu Precipitation, AOGS 11th Annual Meeting, Sapporo, Japan, July 28-August 1, 2014.(Oral)
33. Miyamoto Y., Y. Kajikawa, R. Yoshida, T. Yamaura, H. Yashiro, H. Tomita, Deep Moist Atmospheric Convection in a Sub-kilometer Global Simulation, AOGS 11th Annual Meeting, Sapporo, Japan, July 28-August 1, 2014.(Oral)
34. Nishizawa S., H. Yashiro, Y. Sato, T. Yamaura, S. A. Adachi, R. Yoshida, Hirofumi Tomita, and Team SCALE, Our activity for next generation meteorological simulations in future HPC systems, Joint Workshop of 6th International Workshop on Global Cloud Resolving Modeling and 3rd International Workshop on Nonhydrostatic Numerical Models, Kobe, Japan, September 24-26, 2014.(Oral)
35. Sato Y., Y. Miyamoto, S. Nishizawa, H. Yashiro, Y. Kajikawa, H. Tomita, Transition from cumulus under stratocumulus to isolated cumulus simulated in a single calculation domain,

Joint Workshop of 6th International Workshop on Global Cloud Resolving Modeling and 3rd International Workshop on Nonhydrostatic Numerical Models, Kobe, Japan, September 24-26, 2014.(Oral)

36. Yoshida R., An Impact of Vertical Grid Arrangement in Baroclinic Wave Test, Joint Workshop of 6th International Workshop on Global Cloud Resolving Modeling and 3rd International Workshop on Nonhydrostatic Numerical Models, Kobe, Japan, September 24-26, 2014.(Poster)
37. Adachi S. A., Impact of urban parameters in an urban canopy scheme on urban climate simulation, Joint Workshop of 6th International Workshop on Global Cloud Resolving Modeling and 3rd International Workshop on Nonhydrostatic Numerical Models, Kobe, Japan, September 24-26, 2014.(Poster)
38. Miyamoto Y., Deep Moist Atmospheric Convection in a Sub-kilometer Global Simulation , Joint Workshop of 6th International Workshop on Global Cloud Resolving Modeling and 3rd International Workshop on Nonhydrostatic Numerical Models, Kobe, Japan, September 24-26, 2014.(Poster)
39. Miyamoto Y., A linear thermal stability analysis of discretized fluid equations, Joint Workshop of 6th International Workshop on Global Cloud Resolving Modeling and 3rd International Workshop on Nonhydrostatic Numerical Models, Kobe, Japan, September 24-26, 2014.(Poster)
40. Yashiro H., H. Tomita, M. Satoh, Recent computational performance and scalability of NICAM: toward to the exa-scale computing, Joint Workshop of 6th International Workshop on Global Cloud Resolving Modeling and 3rd International Workshop on Nonhydrostatic Numerical Models, Kobe, Japan, September 24-26, 2014.(Poster)
41. Miyamoto Y., R. Rotunno, G. H. Bryan, Developing an analytical model of maximum potential intensity for tropical cyclones incorporating the effects of ocean mixing, Third Capacity Building Workshop of the WMO/IOC Data Buoy Cooperation Panel (DBCP) for the North Pacific Ocean and Its Marginal Seas (NPOMS-3), Kyoto, Japan, October 6-8, 2014.(Oral)
42. Terai M., H. Yashiro, K. Sakamoto, S. Iga, H. Tomita, M. Satoh, K. Minami, Performance Optimization and Evaluation of a Global Climate Application Using a 440m Horizontal Mesh on the K Computer, SC14, New Orleans, LA, USA, November 16-21, 2014.(Poster)
43. Kajikawa Y., Y.-W. Seo, K.-S. Yun, K.-J. Ha and R. Johnson, Role of the SST Over the East China Sea in the Linkage Between East Asian Winter and Summer Monsoon Variability, AGU fall meeting, San Francisco, CA, USA, December 15-19, 2014.(Oral)
44. Ma X., T. Yoshikane, M. Hara, S. A. Adachi , Y. Wakazuki, H. Kawase, F. Kimura, A comparison of river discharge calculated by using a regional climate model output with

different reanalysis datasets in 1980s and 1990s, AGU Fall meeting, San Francisco, CA, USA, December 15-19, 2014.(Poster)

45. Hara M., S. A. Adachi , H. Kusaka, F. Kimura, Future change of wintertime urban heat island intensity over Japan, AGU Fall meeting, San Francisco, CA, USA, 15-19 Dec 2014.(Poster)
46. Adachi S. A., M. Hara, X. Ma, F. Kimura, Impact of urban parameters in an urban canopy scheme on urban climate simulation, 5th AICS international symposium, Kobe, Japan, December 8-9, 2014.(Poster)
47. Yoshida R., H. Yashiro, H. Tomita, An Impact of Vertical Grid Arrangement in Baroclinic Wave Test, 5th AICS international symposium, Kobe, Japan, December 8-9, 2014.(Poster)
48. Sato Y., Transition from cumulus under stratocumulus to isolated cumulus simulated in a single calculation domain, 5th AICS international symposium, Kobe, Japan, December 8-9, 2014.(Poster)
49. Miyamoto Y., Y. Kajikawa, R. Yoshida, T. Yamaura, H. Yashiro, H. Tomita, Deep Moist Atmospheric Convection in a Sub-kilometer Global Simulation , 5th AICS international symposium, Kobe, Japan, December 8-9, 2014.(Poster)
50. Kajikawa Y., Long term variability of the Asian monsoon onset, Asian monsoon Hydroclimate - Review of MAHASRI and Beyond -, Nagoya, Japan, March 4-5, 2015.(Oral)
51. Kusaka H., A. Suzuki-Parker, T. Aoyaghi, S. A. Adachi , Y. Yamagata, Urban Climate Projection in Tokyo for the 2050’s August by the 4-km horizontal grid spacing RCMs: Impact of RCM and Urban Scenario, 2nd International UGEC Conference, Taipei, Taiwan, November 6-8, 2014.(Poster)
52. 佐藤陽祐、西澤誠也、八代尚、宮本佳明、富田浩文, 将来 HPC での使用を見据えた共通基盤ライブラリ(SCALE)の開発と SCALE を用いて作成されたデータセット, 日本地球惑星科学連合 2014 年大会, 横浜（開港記念会館・情報文化センター）, April 28-May 2, 2014.(Poster)
53. 佐藤陽祐、西澤誠也、八代尚、宮本佳明、富田浩文, 境界層雲の数値実験に雲微物理スキームが及ぼす影響評価, 日本気象学会 2014 年度春季大会, 横浜（開港記念会館・情報文化センター）, May 21-24, 2014.(Oral)
54. 宮本佳明、伊藤純至、西澤誠也、富田浩文, 離散系における線形安定性解析, 日本気象学会 2014 年度春季大会, 横浜（開港記念会館・情報文化センター）, May 21-24, 2014.(Poster)
55. 吉田龍二、八代尚、富田浩文, 傾圧波実験における鉛直格子感覚の影響評価, 日本気象学会 2014 年度春季大会, 横浜（開港記念会館・情報文化センター）, May 21-24, 2014.(Poster)
56. 梶川義幸、山浦剛、富田浩文、佐藤正樹, NICAM で再現された 2012 年のインドモン

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57. 足立幸穂、梶川義幸、西澤誠也、吉田龍二、八代尚、富田浩文, 神戸市と周辺地域の降水イベントを対象とした高解像度再現実験, 日本気象学会 2014 年度春季大会, 横浜（開港記念会館・情報文化センター）, May 21-24, 2014.(Poster)
58. 西澤誠也、八代尚、佐藤陽祐、宮本佳明、山浦剛、富田浩文, LES における格子アスペクト比に対する境界層乱流の依存性, 日本気象学会 2014 年度春季大会, 横浜（開港記念会館・情報文化センター）, May 21-24, 2014.(Oral)
59. 八代尚, OpenACC を用いた全球雲解像モデル NICAM 力学コアの GPU 最適化, GPU Technology Conference Japan 2014, 東京(東京ミッドタウンホール), Jul7 16, 2014.(Oral)
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61. 山浦剛、冨田智彦, 梅雨, NICAM AMIP-like データ利用研究会, 横浜(海洋研究開発機構横浜研究所), August 5, 2014.(Oral)
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65. 佐藤陽祐、西澤誠也、八代尚、宮本佳明、梶川義幸、富田浩文, 広領域・高解像度 LES による層積雲から積雲への遷移過程の再現実験, 日本気象学会 2014 年度秋季大会, 福岡(福岡国際会議場), October 21-23, 2014.(Oral)
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(4) Patents and Deliverables

73. Team-SCALE, Scalable Computing for Advanced Library and Environment (SCALE), Version: 0.1.3 (SCALE-LES Version: 4.1.3), http://scale.aics.riken.jp/, 2015.
74. NICAM-Developers, Nonhydrostatic ICosahedral Atmospheric Model dynamical core package (NICAM-DC),Version: 1.1, http://scale.aics.riken.jp/nicamdc/index.html, 2014

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
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3. Research Results and Achievements

3.1 Development of a unified framework for large-scale multiphysics problems

Based on the Building Cube Method (BCM), we have developed a unified solver framework CUBE (Complex Unified Building cubE) for solving large-scale multphysics problems. The framework has a modular design where CUBE provides a core library containing kernel functionalities e.g. a mesh, flow fields and I/O routines. Solvers are then developed on top of the kernel by connecting necessary kernel modules together, forming a "solver" pipeline, describing the necessary steps to solve a particular problem.

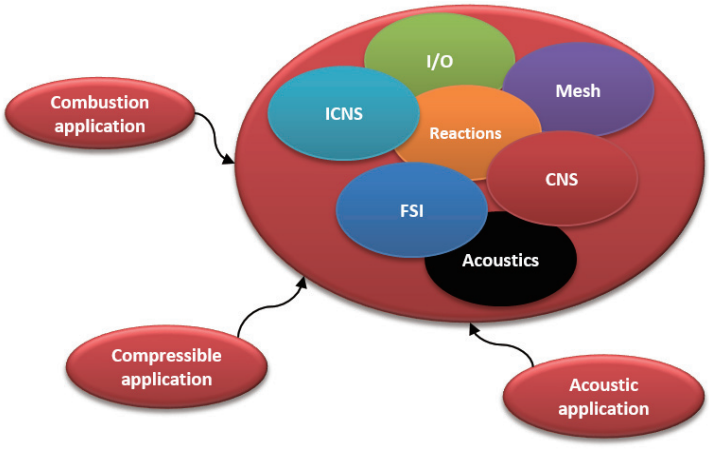
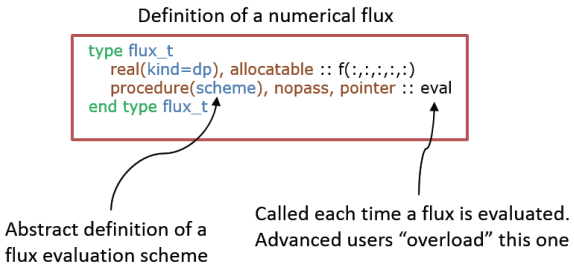


Figure 1. Framework of the unified solver CUBE.

Written in modern Fortran 2003, we have moved towards a fully Object-Oriented abstraction. Where a set of abstract classes defines canonical components of a solver, which is later overloaded by a real solver. Since the framework is targeted to different kinds of users, CUBE's framework already comes with a set of predefined solvers, intended for a general user.



By only providing simulation parameters and geometries, CUBE can be used as a regular flow solver. Advanced users can instead see CUBE as a library. And use it to develop own solvers, tailor-made for a particular application. Similar to other C++ based multiphysics frameworks, CUBE let advanced users overload certain kernel components in their application code. For example, if a user wish to write his own application specific flux evaluation routine, he would only need to overload the base definition of a numerical flux. Once done, the framework will execute the user's code instead of the one in the kernel every time fluxes are evaluated. This way we can keep CUBE's kernel small and general, without application specific code.

One of the recent addition to CUBE is its ability to handle chemical reactions. The current implementation aims towards a DNS/LES formulation, and supports both finite-rate and reduced reaction models as well as several species. In the case of reactive flow, we use a density based formulation and append an additional set of conservation laws to the flow problem.

$$\frac{\partial}{\partial t}\rho + \nabla \cdot (\rho\, u) = 0$$

$$\frac{\partial}{\partial t}\rho u + \nabla \cdot (\rho\, uu) = -\nabla p + \nabla \cdot \tau$$

$$\frac{\partial}{\partial t}\rho e_t + \nabla \cdot \left[\rho\, u \left(e_t + \frac{p}{\rho}\right)\right] = \nabla \cdot (u \cdot \tau) - \nabla \cdot q$$

$$\frac{\partial}{\partial t}\rho\, Y_k + \nabla \cdot (\rho\, Y_k u) = \nabla \cdot (\rho D_k \nabla Y_k) + \dot{\omega}_k$$

Figure 2. Navier-Stokes equations for a multi-species reactive mixture.

Here we have also strived for a general implementation, and have implemented most routines related to flow problems to handle both reactive and non-reactive flow. The kernel does not contain any reaction itself. Instead a user has to describe each reaction by himself in his application code and overload corresponding dummy reactions inside the framework.

Reactive flow is still under heavy development but an early example of this new feature is demonstrated below for a freely propagating premixed flame. Here the unit cube is filled with a fuel+air mixture, and one of the sides is heated in order to ignite the mixture.

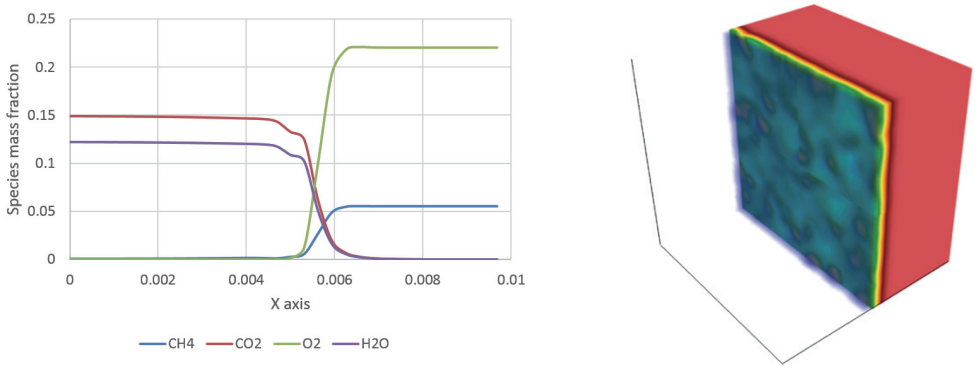


Figure 3. Species mass fraction (left) and Methane consumption at flame front (right).

As can be seen in Fig. 3, once the ignition process starts fuel is completely consumed and replaced with burnt products. Next year our aim is to continue this work and extend it to support reactive flow around as well as inside complex geometries.

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

The new software framework CUBE has been developed through this year, by conjunction with incompressible code which developed last year to realize the analysis in a real development process on the massively parallel environment, including pre- and post-processing.

We received a production vehicle CAD data from Mazda Motor Corporation and it's wind tunnel measurement data. The vehicle type is SUV which is relatively difficult to evaluate because it has large space in engine bay and narrow flow path within small parts affects the entire flow change acting on outside, especially under floor flow and grill opening drag.

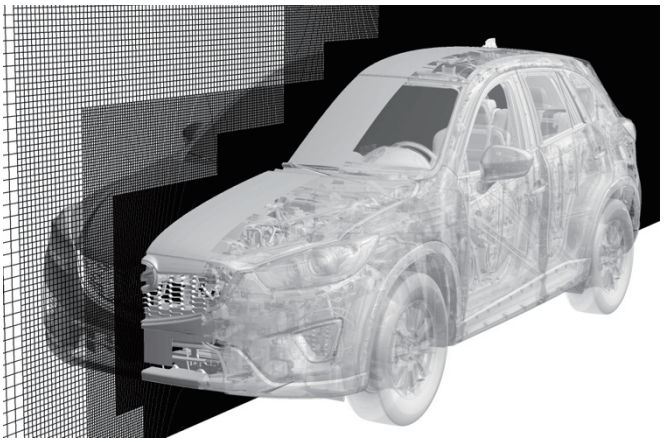


Figure 4. Overview of computational grid and geometry (provided by MAZDA Motor Company).

Figure 5. Flow visualization results of vortex structure

We have conducted basic validation of aerodynamic performance comparing with total pressure flow field which obtained by measurement. The typical flow characteristics especially longitudinal vortex structure around under floor, A-pillar vortex in wake region, side wake structure passed through front wheel arch has successfully reproduced. But, it was difficult to get high accurate results on the total drag force prediction because of the difficulty of integration on 'dirty' geometry data which is required to improve. To show the applicability on large scale analysis, we have conducted demonstration case using 27 billion numerical cells. Unfortunately we couldn't run it enough longer to obtain the converged result due to the shortage of calculation resource, but MAZDA could decide to promote the results inside their organization, and continue the current research activity using our software in FY2015 by submitting the application and accepted the industrial use project on K-computer.

In addition, we have joined a research activity on Wind-HPC consortium which is organized by Tokyo Institute of Technology and several Japanese major construction companies. And provided our software. They are accepted the general use project on K-computer. The purpose of this project is to obtain accurate prediction on the wind pressure acting on building with a complicated shape, and very fine Cartesian grid. The actual urban area geometry has provided that is including housings, buildings, vegetation, and street, and so on. Then we provided a quick results using LES using very fine grids with large scale simulation for several are in Tokyo, then evaluated the turbulence characteristics on canopy and developed utilities to utilize the input boundary conditions on scale cascading condition. Finally, we have summarized the results to publish, it is still on going, and could get an upcoming post-K computer project regarding wind environment evaluation for building construction on severe climate condition.

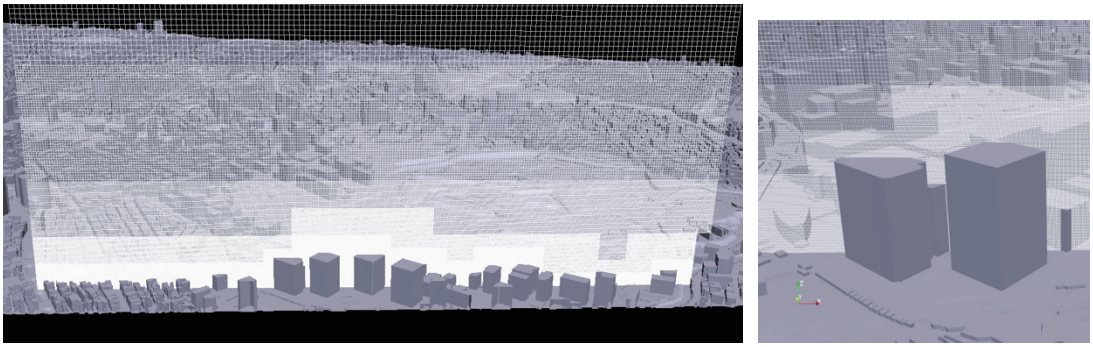


Figure 6. Overview of computational grid for wind environment analysis around Tokyo station area.

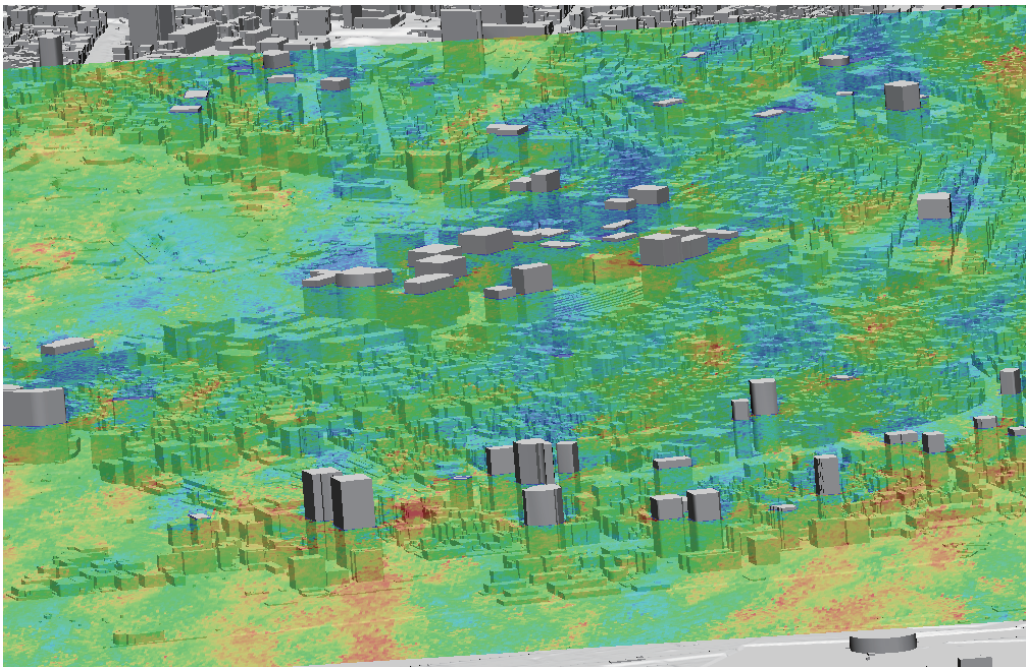


Figure 7. Example of the flow field results around Tokyo bay area.

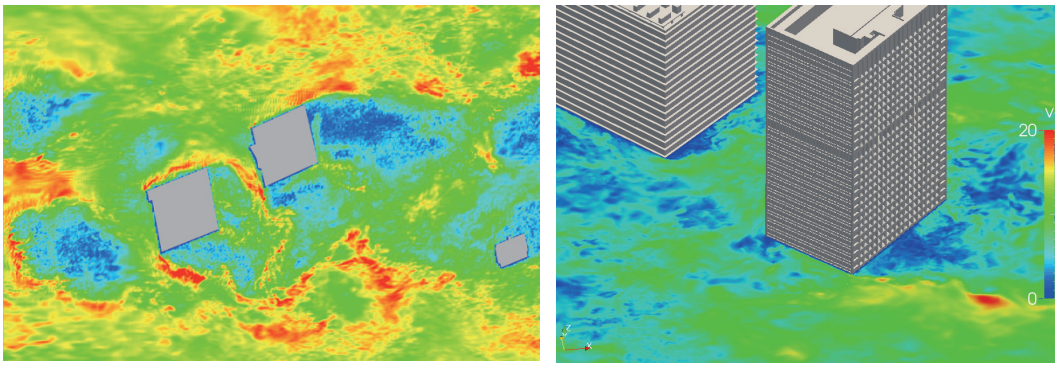


Figure 8. Detailed flow result showing specific building, showing the interaction of vortex and structure.

[1] Onishi, K., Tsubokura, M., Obayashi, S., and Nakahashi, K., "Vehicle Aerodynamics Simulation

for the Next Generation on the K Computer: Part 2 Use of Dirty CAD Data with Modified Cartesian Grid Approach," SAE Int. J. Passeng. Cars - Mech. Syst. 7(2):528-537, 2014, doi:10.4271/2014-01-0580.

[2] Onishi, K., Tsubokura, "Large-scale Simulation of Full Vehicle Aerodynamics using Cartesian Grid Approach optimized on K-computer", JSAE Paper Number: 20145232, No.24-14, 2014.

[3] Onishi, K., Tsubokura, M., Obayashi, S., and Nakahashi, K., "Practical applications for the computational vehicle aerodynamics on the massively parallel supercomputer: Part 2, hierarchical cartesian grid approach utilizing dirty CAD data", proceedings of 11th World Congress on Computational. Mechanics (WCCM XI). July 21, 2014, Barcelona, Spain.

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[6] Tamura,T., Nozu, T., Tsubokura, M., and Onishi, K.,"LES of turbulent boundary layer flow over urban-like roughness elements", 67th Annual Meeting of the APS Division of Fluid Dynamics, Volume 59, Number 20, 2014, BAPS.2014.DFD.L25.5.

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

Aeroacoustics is one of the most important subjects in industrial applications such as vehicle aeroacoustics, fan noise in electronic devices and jet noise reduction … etc. In order to use the unified program developed by our team on this kind of topics to help industries to control the noise, the adaptability for turbulent flows, absorbing boundary condition to obtain accurate results, and immersed boundary condition for complex geometry have been developed and validated.

Fig. 9 shows the comparison of normalised turbulence intensities with the results of Kim [1] done by direct numerical simulation (DNS). It is indicated that under the condition of $\Delta t^+ < 0.32$, our numerical scheme can accurately capture the turbulence phenomena. Through this study, the adaptability for turbulent flows of our numerical scheme is validated and the guide line of the parameters is also builded. The present results have been published in International Journal of Computational Fluid Dynamics [2].

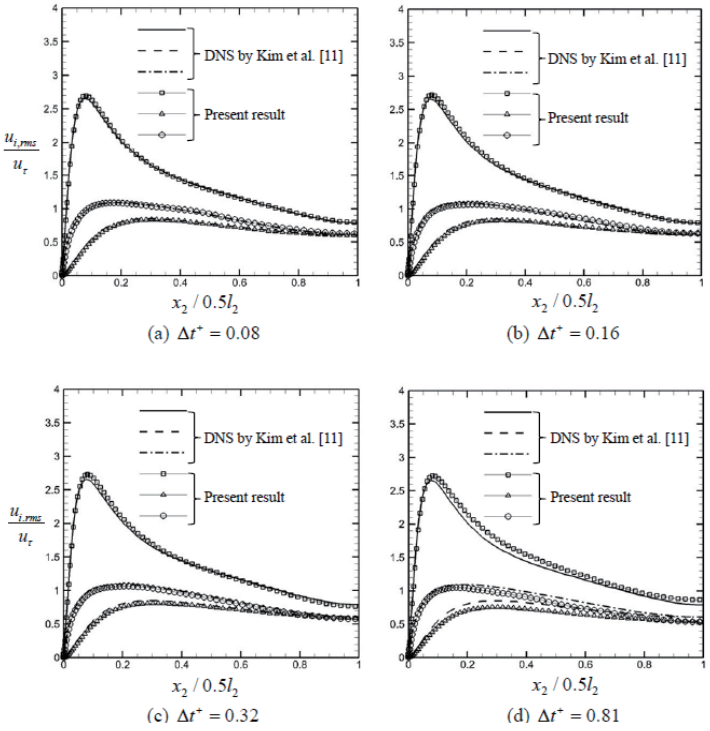
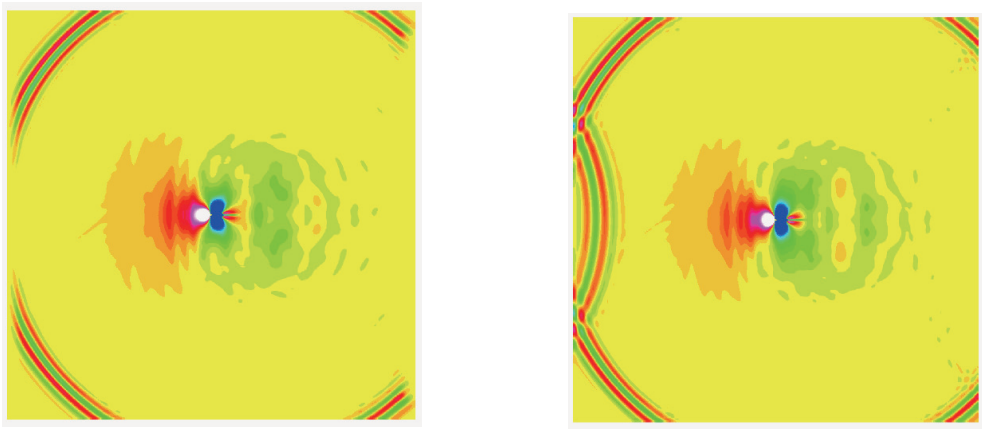


Figure 9. The comparison of normalised turbulence intensities with the results of Kim [1].

[1] Kim J, Moin P and Moser R, Turbulence statistics in fully developed channel flow at low Reynolds number, J. Fluid Mech. (1987) 133-166.

[2] C. G. Li, M. Tsubokura and K. Onishi, Feasibility investigation of compressible direct numerical simulation with a preconditioning method at extremely low Mach numbers, Int. J. Comput. Fluid Dyn. (2014) 411-419.

Because the order of the difference for the pressure between the aeroacoustic field and flow field is very large, the special treatment for the boundary is necessary to prevent the pollution on the aeroacoustic field. The absorbing boundary has been developed to handle the above issue. Fig. 10 shows the pressure fluctuation propagation across the boundary. In Fig 10(a), because the absorbing boundary is added in the left side, the pressure fluctuation can leave the computational domain without any reflection. On the other hand, in Fig 10(b), due to the lack of the absorbing boundary, the reflection of the pressure fluctuation affects the field.



(a) With absorbing boundary (b) Without absorbing boundary

Figure 10. The pressure fluctuation propagation.

With adaptability for turbulent flows and absorbing boundary condition, acoustic on a cascade of flat plate has been conducted. Owing to the complex phenomena and mechanism of the acoustic, the numerical scheme with high accuracy and immersed boundary condition for compressible flow are needed to capture the interaction of the pressure fluctuation between acoustic field and flow field. Fig. 11 shows the Instantaneous pressure fluctuation magnitude. The acoustic pressure is radiated from the plate can be clearly observed and the pressure fluctuation propagation can be well captured.

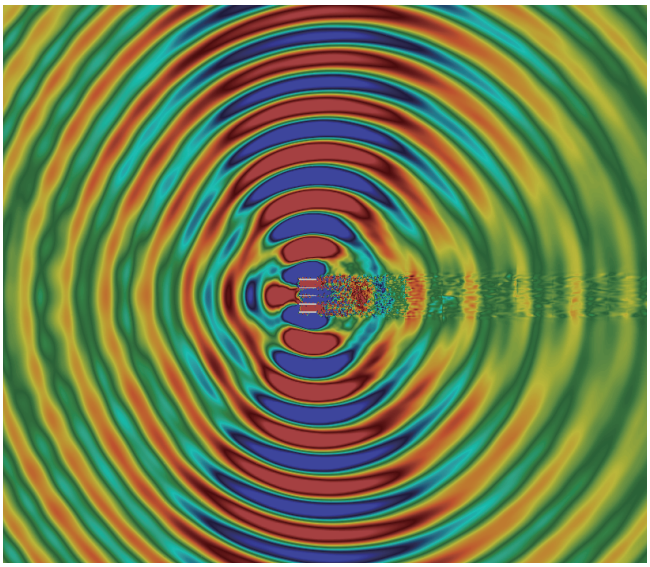


Figure 11. Pressure fluctuation

Based on the present results mentioned above, the computational aeroacoustic (CAA) on the vehicle will be conducted for the next year. Fig. 12 shows the preliminary results

performed by the compressible program. The flow field around the whole car is simulated and the complex geometry of the car be well presented.

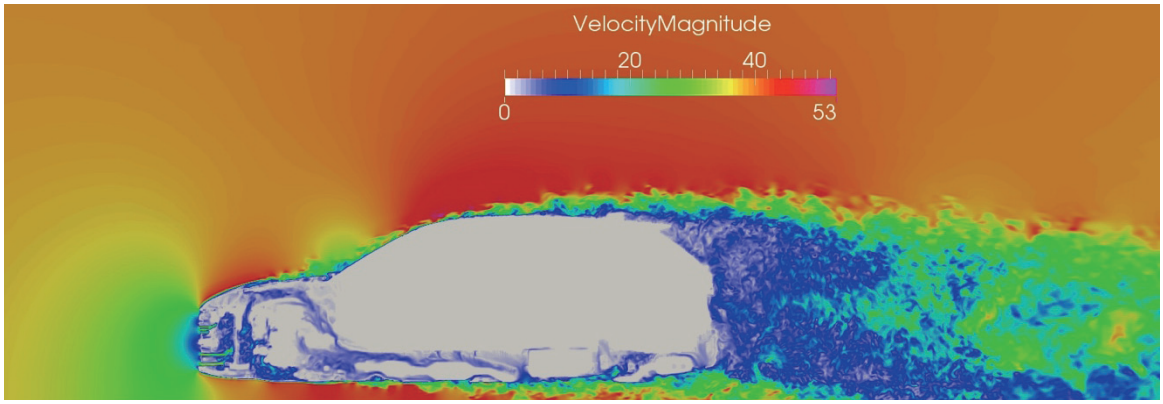


Figure 12. Velocity magnitude

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.

A fully Eulerian (FE) and Lagrangian-Eulerian based immersed boundary method (IBM) was implemented and tested. Through the FE-IBM we were able to obtain promising results with small-scale test cases in FY13. As was pointed out in the last report in FY13, the key limitation/drawback of the fully Eulerian based method is in the lack of its ability to accurately capture and maintain the original shape of the structure. This limitation of the fully Eulerian methods can partially be alleviated by using higher order advection schemes for the colour function that is used to represent the structure. In the case where the colour function is a level set, the limitation can be further alleviated through the reinitialization process. The higher order advection schemes, and the reinitialization process in the case of level set, are able to represent the shape of structures that have simple geometries with no sharp changes in curvature (eg. a sphere, torus, etc.). But, for more complex real-world geometries, which involve sharp changes and discontinuities in curvature, the ability of FE methods to retain original shape over time is lacking. The maintenance of the shape of the structure over time is limited by the grid scale and numerical diffusion. While the numerical diffusion can be reduced by higher order schemes, the grid resolution necessary for accurately representing and maintaining the shape of the structure is prohibitively small.

Owing to the limitation of FE methods for IBM discussed above, it was decided that the capabilities and limitations of Lagrangian-Eulerian (LE) based IBM need to be reassessed. The two main

limitations of LE approach and possible resolution of these limitations are discussed below.

I. LE methods involve expensive interpolation operators between the Lagrangian mesh and the Eulerian mesh.

The interpolation between Lagrangian and Eulerian meshes, for a given point on the Lagrangian mesh, involves searching a set of nearest neighbouring Eulerian mesh points. It is this searching operation that makes the interpolation expensive. To overcome this limitation we have developed a *Lagrangian BCM data structure*. This new data structure eliminates the 'search' step of the interpolation. The nearest set of Eulerian neighbours are now located by simple inexpensive *arithmetic operations* rather than expensive search operations. The *Lagrangian BCM data structure* has been recently added to the code with the unified framework: Complex Unified Building cubE method (CUBE)

II. Moving structures involve moving Lagrangian meshes which increases the difficulty of load balancing.

A dynamic load balancing method has been implemented in the Unified BCM framework (CUBE). The dynamic load balancing technique in use can easily be modified to account for a mobile Lagrangian mesh. This is done by assigning a larger weight to BCM cubes with Lagrangian mesh during grid partitioning.

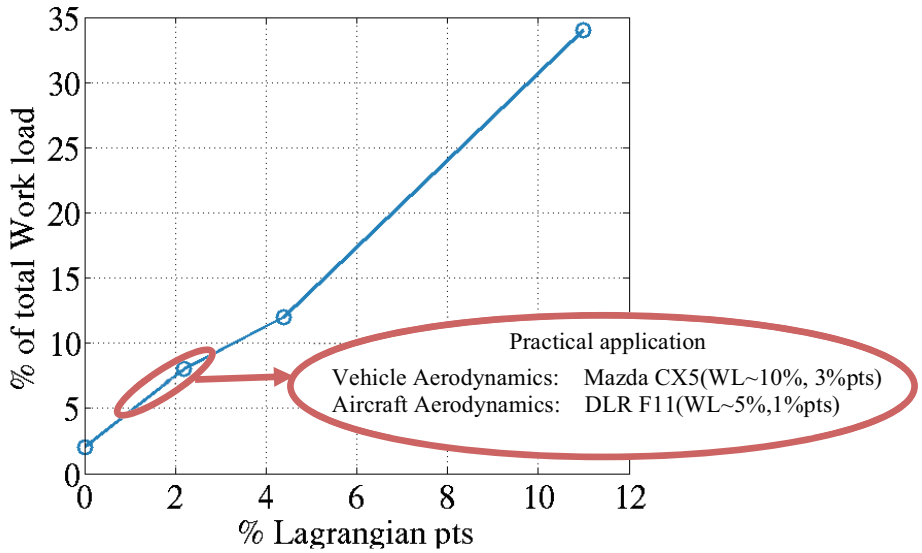


Figure 13. Profiling data for LE based IBM. Percentage of total time spent on Lagrangian operations plotted against proportion of Lagrangian points relative to BCM mesh size, i.e (No. Lagrangian pts)/ (BCM mesh size) * 100.

Reinit Iterations	**20**	**50**	**100**	**200**
% Work Load	9	19	32	48

Table 1. A comparison of percentage time spent on reinitialization of the level set for increasing reinitialization iterations (Note: These are crude extrapolated estimates.).

Performance comparison LE vs FE: Fig. 13 shows the results of performance evaluation of LE based IBM solver. In the figure percentage work load (WL) is plotted against proportion of Lagrangian points relative to the number of Eulerian mesh points (BCM mesh size). The work load ranges from 2% for 0.01% Lagrangian points to 34% for 10% Lagrangian points. The Lagrangian-Eulerian approach is practical only if the WL of Lagrangian operations is less than 20%. Real world applications of interest to our research are vehicle aerodynamics, aircraft aerodynamics, urban flow dynamics, etc. As is highlighted, in Fig. 13 for practical application of interest the percentage of Lagrangian points ranges from 1% to 4%.; for proportion of Lagrangian points in this range, the work load ranges from 5% to 12%. We believe that this amount for work load for the Lagrangian is reasonable for practical applications.

In Table 1 we present the performance analysis of Fully Eulerian based IBM solver, where the structure is represented by a level set function. As alluded to above, level set undergoes distortion due to motion of the structure and numerical diffusion. This distortion has to be corrected at every time step of the solver, which is done through the reinitialization process. Reinitialization is an iterative process that is carried out until the level reaches the desired state (in our case, accurate representation of the shape of the structure). The number of iterations necessary for the level set to reach the desired state depends on several factor, namely: complexity of the geometry, problem size, etc. For simple geometries like a sphere, the iteration necessary are of the order of O(10), more complex geometries like a vehicle the number is of the order of O(100). The work load of the reinitialization ranges from 9% to 48% for 20 to 200 iterations. For most practical applications, anywhere between 20 to 100 iterations would necessary, the load corresponding to these iterations ranges between 9% to 30%.

Despite our a priori expectation that a Fully Eulerian approach would be computationally less expensive, we find that the Lagrangian based approach has a slight edge over Fully Eulerian approach.

[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

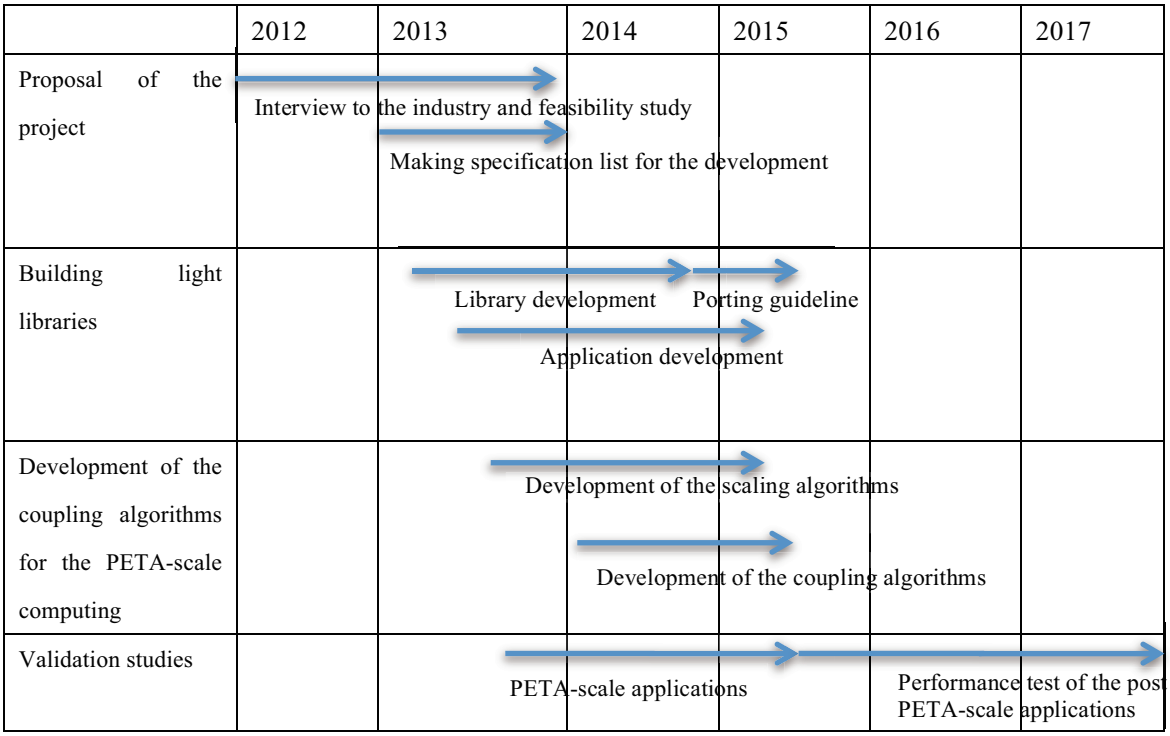
b. Proposal of the technological trend of HPC simulation toward EXA-scale

(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



5. Publication, Presentation and Deliverables

(1) Journal Papers

1. Makoto Tsubokura, Andrew Hamilton Kerr, Keiji Onishi, Yoshimitsu Hashizume: Vehicle Aerodynamics Simulation for the Next Generation on the K-computer: Part 1 Development of the framework for fully unstructured grids up to 10 billion numerical elements, SAE International Journal of Passenger Cars – Mechanical Systems, 7(2): 2014-01-0621(2014)
2. Keiji Onishi, Makoto Tsubokura: Vehicle Aerodynamics Simulation for the Next Generation on the K computer: Part 2 Use of Dirty CAD Data with Modified Cartesian Grid Approach, SAE International Journal of Passenger Cars – Mechanical Systems, 7(2): 2014-01-0580(2014)

3. Chun-Gang Li, Makoto Tsbuokura, Keiji Onishi: Feasibility Investigation of Compressible Direct Numerical Simulation with Preconditioning Method at Extremely Low Mach Numbers, International Journal of Computational Fluid Dynamics, vol.28, Issue 6-10, pp.411-419 (2014)
4. 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.
5. 坪倉誠，大西慶治：HPC-LES を活用した自動車用数値風洞の開発，ターボ機械（ターボ機械協会誌），vol.42, No.5, pp.36（324）-43（325）（2014）
6. 坪倉誠，大西慶治：自動車の大規模空力シミュレーション　―非構造格子 vs. 構造格子―，情報処理（情報処理学会誌），vol.55, No.8, pp.823-828 (2014)

(2) Conference Papers

7. **Makoto Tsubokura**, Ryuya Kobayashi, Shoya Ota, Shinji Okamine, Kinzan Ryu, Toshio Onuma, Nobuhiro Sasuga: The Effect of Wheel Geometry on the Total Aerodynamic Drag of a Road Vehicle, 32nd AIAA Applied Aerodynamics Conference (16-20, June, 2014, Hyatt Regency Atlanta, Altanta, GE), AIAA-2014-3126 (2014)
8. Kohei Nara, **Makoto Tsubokura**, Jun Ikeda: A Numerical Analysis of Unsteady Aerodynamics of Formula Car during Dynamic Cornering Motion, 32nd AIAA Applied Aerodynamics Conference (16-20, June, 2014, Hyatt Regency Atlanta, Altanta, GE), AIAA-2014-3138 (2014)
9. Jing Li, **Makoto Tsubokura**, Masaya Tsunoda: Numerical Investigation of Drag Crisis of a Sphere and the Effect of Surface Roughness, 10th International ERCOFTAC Symposium on Engineering Turbulence Modelling and Measurements (17-19, September, 2014, Don Carlos Resort, Marbella, Spain)
10. Keiji Onishi, **Makoto Tsubokura**: Optimized preprocessing of tens of billions of grids in a full-vehicle aerodynamic simulation on the K-computer, Proceedings of the 2014 International Vehicle Aerodynamics Conference (14-15, October, 2014, Holywell Park, Loughborough, Great Britain), pp.149-158 (2014)

(3) Invited Talks

11. 坪倉誠：「京」が拓いた新たなものづくり　～自動車空力設計を例に～, 未来をひらくスーパーコンピュータ　～「京」からその先へ限りなき挑戦～（理研計算科学研究機構、高度情報科学技術研究機構主催）（2014 年 8 月 23 日、24 日、科学技術館、東京）
12. 坪倉誠 : HPC-CFD が拓く自動車空力シミュレーション :（2014 年 12 月 19 日、JAXA

相模原キャンパス）

(4) Posters and presentations

13. Andrew H. Kerr, Keiji Onishi, **Makoto Tsubokura**: Practical Applications for the Computational Vehicle Aerodynamics on the Massively Parallel Supercomputer: Part 1, Framework for the Fully Unstructured Finite Volume Cells, 11th World Congress on Computational Mechanics (WCCM XI), July 20-25, 2014, Barcelona, Spain (2014)
14. Keiji Onishi, **Makoto Tsubokura**, Shigeru Obayashi and Kazuhiro Nakahashi: Practical Applications for the Computational Vehicle Aerodynamics on the Massively Parallel Supercomputer: Part 2, Hierarchical Cartesian Grid Approach Utilizing Dirty CAD Data, 11th World Congress on Computational Mechanics (WCCM XI), July 20-25, 2014, Barcelona, Spain (2014)

(5) Patents and Deliverables

HPC Programming Framework Research Team

1. Team members

Naoya Maruyama (Team Leader)
Motohiko Matsuda (Research Scientist)
Shinichiro Takizawa (Research Scientist)
Mohamed Wahib (Postdoctoral Researcher)
Koji Ueno (Student Trainee)
Satoshi Matsuoka (Senior Visiting Scientist)
Tomoko Nakashima (Assistant)
Aya Motohashi (Assistant)

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. We also study high performance graph analytics on the K computer. 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 has been developed over the last several years, is similar to the original MapReduce design by Dean and Ghemawat, but its implementation is significantly extended for the node and storage architectures of large-scale supercomputers such as the K computer. Highlights of new development and features are summarized below.

2) Automated Program Transformation for Better Access Locality

One of the important architectural trends is the deeper memory hierarchy consisting of different types of on-chip and off-chip memories with different capacity and performance profiles. To exploit the increase of the processor compute performance, it is becoming more important to effectively exploit near-processor faster memories by taking advantage of any available data access locality. General-purpose optimizing compilers are equipped with advanced program transformations to

address the challenge, however, they are often limited to a small set of rather simple program codes. We addressed the problem in the context of stencil computations on GPUs. More specifically, we have developed an automated framework that optimizes a given user CUDA programs by fusion and fission of CUDA kernels.

3) High Performance Graph Analytics Study with Graph500

Graph analytics is a new class of applications that are increasingly more important in various domains of sciences and societies. However, solving large-scale graph analytics problems is highly challenging due to its strong demand on computational and storage capability and capacity. The K computer, being the forth-fastest machine with Top500, is potentially able to serve such demand, however, the more unstructured characteristics of both computations and data accesses in graph analytics than those in conventional structured simulation codes require detailed attentions to be paid to different aspects of performance analyses and optimizations. As a first case study, we have been evaluating and optimizing the Graph500 benchmark for the K computer.

3. Research Results and Achievements

3.1. KMR (K MapReduce)

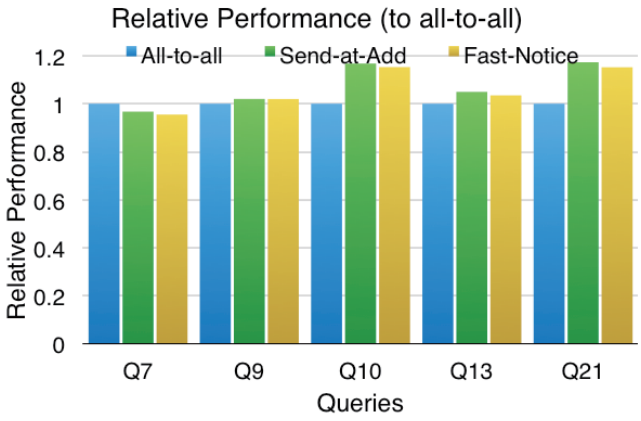
We are working on achieving highly reliable, high performance and high productivity data processing framework for large scale supercomputing systems, especially for the K computer. To this end, we achieved the following five research/development achievements. All these achievements are implemented in our MapReduce framework named KMR (K MapReduce).

1) Evaluation of asynchronous communication in MapReduce

KMR is designed to exploit the capacity and capability of supercomputers. To match the super-computer environment, KMR runs on memory, communicates by MPI, and utilizes CPU cores by multithreading. In such a design, the natural choice of shuffling communication is a collective communication MPI_Alltoallv. However, collective communications are synchronous and thus cannot exploit overlapping of communication and computation, which have been demonstrated effective in other MapReduce systems in the literature. Although overlapping would appear to be effective over collectives at first glance, handling MPI requests needed in overlapping takes cost in proportion to the number of processes. The cost hinders the performance especially in large scale, while the collectives are very efficient in large scale. This research evaluates the effectiveness of overlapping versus collective communications.

For this purpose, two new modes of shuffling communication are introduced in addition to the normal all-to-all mode. In the send-at-add mode, messages are sent when the buffer is full during mapping and reducing. In the fast-notice mode, a lightweight event notification is performed

alongside the send-at-add mode messages. We chose TPC-H as a benchmark with a shuffle-heavy workload, and benchmarked five out of the 22 queries defined in TPC-H. This benchmark was performed with 1024 nodes on the K Computer.

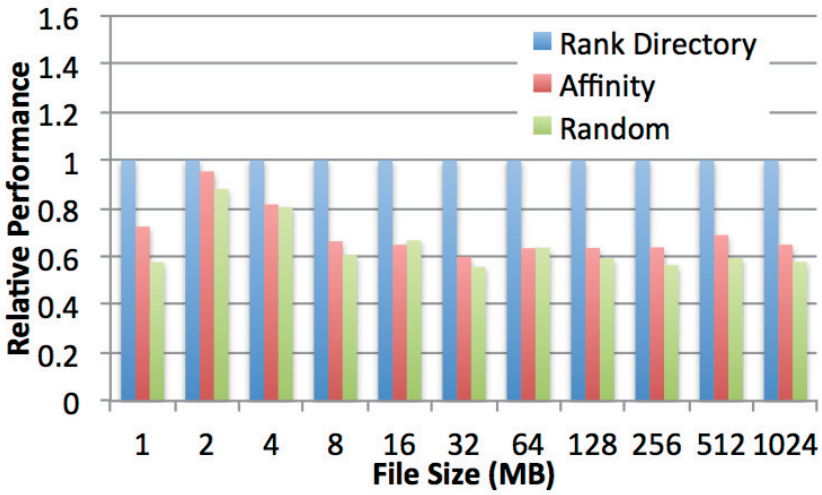


The results show only a slight improvement by overlapping, at most 15% reduction of the execution time. Although the fast-notice mode achieves precise polling timing, it slightly degrades the performance. Analyzing the breakdown of completions of the send-at-add mode messages reveals that the mapping/reducing operations are quickly finished before the messages are exchanged. That is, there is a little chance of overlapping for TPC-H queries. We conclude that the benefit of overlapping is marginal in the current MPI environment.

2) Locality-aware task assignment for improving IO performance

Files in a supercomputing system are stored in shared parallel filesystems, and when these files are used as inputs for a data processing job that uses thousands of compute nodes, these nodes individually but sometimes simultaneously access their inputs. This behavior can raise heavy IO contention on the shared parallel filesystem. We propose a task assignment method that considers locations of tasks' files and distance between the files and nodes to minimize the distance and reduce the IO contention for MapReduce's map task execution phase where such an IO pattern occurs. To implement this method for the K computer, we identify the six dimensional coordinates of nodes and location of file servers that stores each file, and then map nodes and tasks so that IO distance will be minimized.

We performed a simple file read task execution benchmark using K's shared parallel filesystem and rank directory, which is a process local directory. Though our proposal achieves only 70% of performance against rank directory where users explicitly need to specify task and node mappings, it improves 7% of performance against random task assignment [4-1].

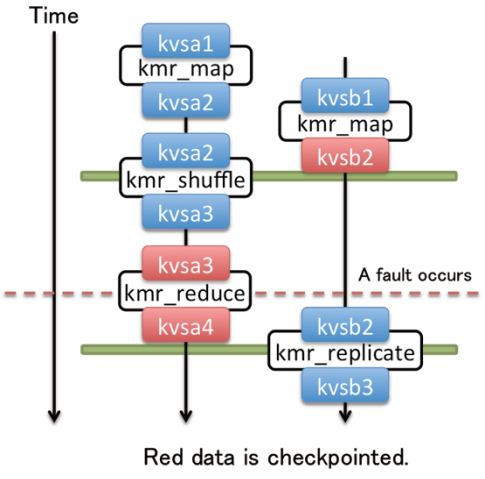


We also conducted an evaluation using a genome sequence-mapping program where 1,173 mapping tasks are simultaneously executed on 1,152 nodes. As a result, the average time of executing a task of our proposal is 870.75 seconds and that of the random task assignment is 882.05 seconds, 2% of performance improvement.

3) Checkpoint/Restart

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 mechanism to KMR (KMRCR) in FY2013. Users can easily and transparently use KMRCR only by setting an environmental variable.

```
kvsa1 = kmr_create_kvs()
kvsa2 = kmr_create_kvs()
kvsa3 = kmr_create_kvs()
kvsa4 = kmr_create_kvs()
kvsb1 = kmr_create_kvs()
kvsb2 = kmr_create_kvs()
kvsb3 = kmr_create_kvs()
kmr_map_once(kvsa1)
kmr_map_once(kvsb1)
kmr_map(kvsa1, kvsa2)
kmr_map(kvsb1, kvsb2)
kmr_shuffle(kvsa2, kvsa3)
kmr_reduce(kvsa3,ksva4)
kmr_replicate(kvsb2,kvsb3)
```



However, as a drawback of ease and transparent use and achieving high reliability, KMRCR takes checkpoints of all KMR data and as a result it causes heavy IO load on disk. To reduce IO load, we implement two options to KMRCR. One is "*no fsync*" mode where fsync to a file is not performed until execution is done. This will reduce reliability, but if a user can assume that MTBF of a system

is larger than expected job completion time and there is only software fault, like killing by signal, It may help increasing performance. The other is "*selective*" mode where only user-specified KMR data are checkpointed. This will lose transparency, but also increase performance.

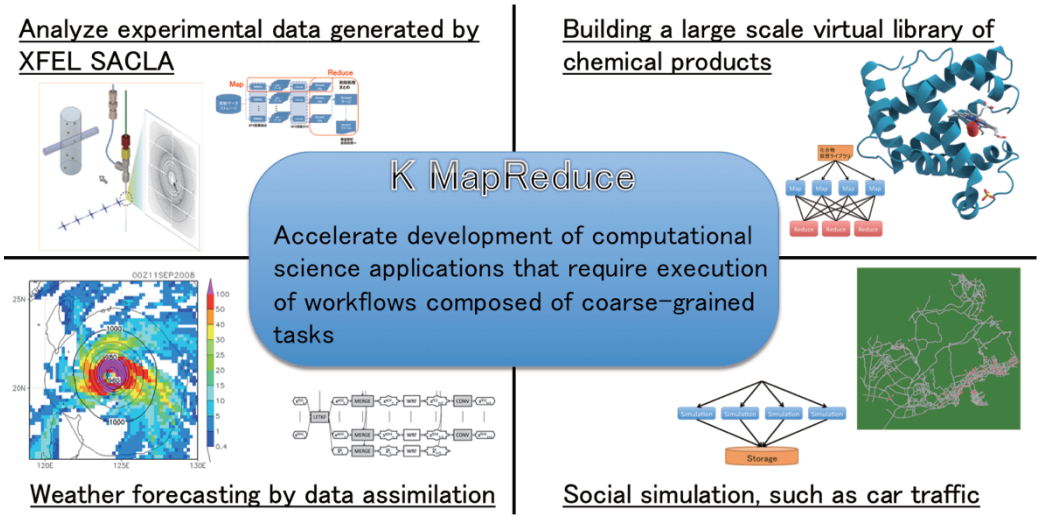
4) KMRRUN: high productive utility for MapReduce job execution

KMR provides C/Fortran API to fully use KMR functions and *kmrshell* utility for programming-less MapReduce execution. *KMRRUN* is a new utility that solves problems that kmrshell has and adds new functions that kmrshell doesn't have: map-only task execution, support for executing MPI program as task and checkpoint/restart.

5) Python API

KMR C/Fortran API enables full access to KMR functions but requires complex programming. On the other hand, using KMRRUN enables ease execution of MapReduce program but lacks flexibility. To achieve both full access to KMR functions and ease programming/executing MapReduce program, we are now designing and implementing Python API for KMR. This is an on-going project and will be release by middle of FY2015.

These above achievements, except the last one, are implemented in KMR and are released as open source software licensed under LGPL-2.1 [5-1]. We released six versions of KMR in FY2014. KMR is already widely used to develop various areas of computational science applications that require execution of workflows composed of coarse-grained tasks, such as large scale data processing and parallel task execution. To further propagate KMR, we hold lectures for KMR twice in this year. There ware 19 attendees in the first lecture and 9 attendees in the second from academia and industry.



3.2 Scalable Kernel Fusion for Memory-Bound Applications

We observed a pattern in a class of stencil-based scientific applications: GPU implementations of some applications relying on finite difference methods can include tens of kernels that are memory-bound. Kernel fusion can improve performance by reducing data traffic to off-chip memory via data reuse. We introduced a problem definition and proposed a scalable method for searching the space of possible kernel fusions to identify optimal kernel fusions for large problems. The proposed method was manually tested on real-world applications and showed promising results [2-3].

As a follow-up, we developed an end-to-end framework for automatically transforming stencil-based CUDA programs to exploit inter-kernel data locality. The CUDA-to-CUDA transformation collectively replaces the user-written kernels by auto-generated kernels optimized for data reuse. The transformation is based on two basic operations, kernel fusion and fission, and relies on a series of automated steps. The framework is modeled to provide the flexibility required for accommodating different applications, allowing the programmer to monitor and amend the intermediate results of different phases of the transformation. We demonstrated the practicality and effectiveness of automatic transformations in exploiting exposed data localities using a variety of real-world applications with large codebases that contain dozens of kernels and data arrays. Experimental results show that the proposed end-to-end automated approach, with minimum intervention from the user, improved performance of six applications with speedups ranging between 1.12x to 1.76x [2-2].

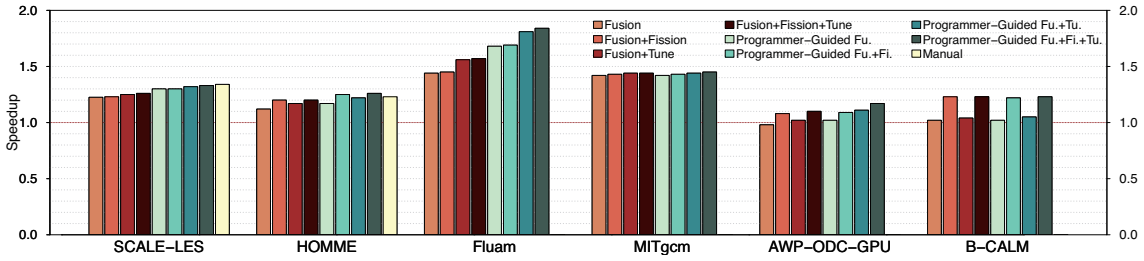


Fig. 1: Nvidia K40 speedup compared to baseline CUDA version for six real-world applications

3.3 High Performance Graph Analytics Study with Graph500

We have extended our implementation of the benchmark several times. Our first extension allowed us to achieve the fastest performance on the Graph500 benchmark list published on June 2014. Our algorithm required the number of nodes to be a power of two, so we used 65536 compute nodes out of more than 80,000 nodes of K. The scale of the system requires highly efficient inter-node parallelization, thus we developed a new algorithm that optimizes inter-node communication using bitmap representations. Furthermore, our algorithm also adaptively uses a sparse vector representation depending on traversal phases. These communication optimizations allowed us to greatly improve the scalability and resulted in 17,977 GTEPS with 65336 nodes for the scale 40 problem of the benchmark. In other words, our highly efficient implementation can traverse an extremely large graph of 1 trillion nodes and 16 trillion edges just under a second. This resulted in the fastest score published on June 2014, followed by the Sequoia system at Lawrence Livermore National Laboratory, which achieved 16,599 GTEPS.

As the second optimization, we have extended the implementation so that an arbitrary number of nodes can be used. While the first version was restricted to 65,536 nodes at maximum, this extension potentially allows us to use as many nodes as 82,944 and to boost the performance by up to 1.2x. However, it can also negatively impact the performance of communication since some of the key MPI communication routines are highly optimized for cases when the number of nodes is a power of two, which is a typical usage pattern in most of scientific simulation codes. As a result, the final performance was 19,585 GTEPS, which resulted in the second rank in the Graph500 list published on November 2014. We observed that the majority of the benchmark time is now spent in communication phases, and are investigating possible optimizations for further performance improvements.

4. Schedule and Future Plan

We plan to continue the development of KMR for 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 plan to release the kernel-fusion framework in the near future. We also plan to extend the methodology to different application domains since memory access performance is almost a ubiquitously important problem. For the graph analytics study, we plan to continue our performance and optimization studies using the Graph500 benchmark.

5. Publication, Presentation and Deliverables

(1) Journal Papers

(2) Conference Papers

1. Motohiko Matsuda, Shinichiro Takizawa, Naoya Maruyama, Evaluation of Asynchronous MPI Communication in Map-Reduce System on the K Computer, EuroMPI Workshop 2014, Kyoto, Japan
2. Mohamed Wahib, Naoya Maruyama, Automated GPU Kernel Transformations in Large-Scale Production Stencil Applications, HPDC'15, ACM Proceedings of the International Symposium on High-Performance Parallel and Distributed Computing, Portland, US
3. Mohamed Wahib, Naoya Maruyama, Scalable Kernel Fusion for Memory-Bound GPU Applications, SC'14, ACM/IEEE Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, New Orleans, US
4. Tetsuya Hoshino, Naoya Maruyama, Satoshi Matsuoka, "An OpenACC Extension for Data Layout Transformation," Proceedings of the First Workshop on Accelerator Programming using Directives (WACCPD '14), New Orleans, LA, November 2014.
5. Kento Sato, Kathryn Mohor, Adam Moody, Todd Gamblin, Bronis R. de Supinski, Naoya Maruyama, Satoshi Matsuoka, "A User-level Infiniband-based File System and Checkpoint Strategy for Burst Buffers," 14th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid'14), Chicago, IL, May 2014.
6. Kento Sato, Adam Moody, Kathryn Mohor, Todd Gamblin, Bronis R. de Supinski, Naoya Maruyama, Satoshi Matsuoka, "Fault Tolerant Messaging Interface for Fast and Transparent

Recovery," 28th IEEE International Parallel and Distributed Processing Symposium (IPDPS'14), Phoenix, AZ, May 2014.

(3) Invited Talks

1. Naoya Maruyama, "Japanese HPC Update: Exascale Research and Next-Genearation Flagship Supercomputer," 3rd Workshop on Extreme-Scale Programming Tools, Keynote Speech, New Orleans, LA, November 2014.
2. Naoya Maruyama, "High Performance and Highly Productive Stencil Framework for GPU Accelerators," International Workshop on Codesign, Invited Talk, Gungzhou, CN, November 2014.

(4) Posters and presentations

1. Shinichiro Takizawa, Motohiko Matsuda, Naoya Maruyama, Towards Locality-aware Large-scale Data Processing, Annual Meeting on Advanced Computing System and Infrastructure (ACSI) 2015, Tsukuba, Japan

(5) Patents and Deliverables

1. Motohiko Matsuda, Shinichiro Takizawa, Naoya Maruyama, "KMR: A MapReduce Library for K", http://mt.aics.riken.jp/kmr/, 2013.
2. No. 1 on the Graph500 Ranking of Supercomputers, June 2014.
3. No. 2 on the Graph500 Ranking of Supercomputers, November 2014.

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 we named “HIVE”, and also to deliver this system to the users. To achieve this aim, we are developing some fundamental technologies essential to build parallel visualization systems for large-scale datasets, and at the same time, are integrating them into the HIVE system. The HIVE system consists of a parallel rendering kernel named “SURFACE”, some peripheral libraries, and a Web-based user-interface. The main idea of the SURFACE is to exploit the sort-last parallel rendering method, which is divided into the following three tasks: data loading, parallel rendering, and image compositing.

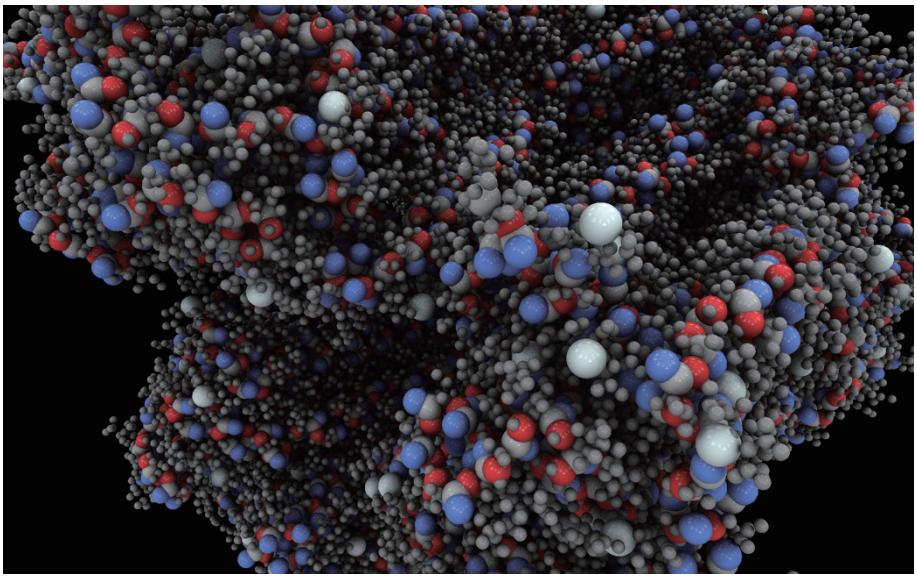


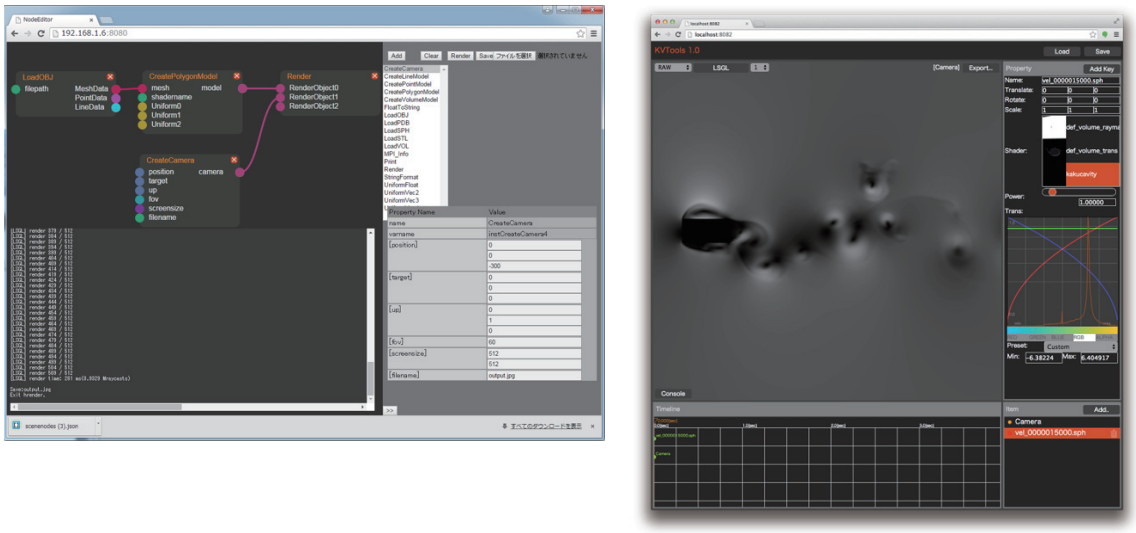
Figure 1. Example of high-quality ray tracing image from a molecular dynamics simulation data. This image was generated using 82,944 nodes on K-Computer.

Although HIVE system is still under development, we have already applied this system to visualize some results from large-scale molecular dynamics simulations executed by other AICS teams. Recent investigations have shown us that the HIVE system enables the users to render more than 10 million atoms on a standard computer resource, and to generate extremely high-resolution images (over 16K resolution) in parallel. Figure 1 shows an example of high-resolution image from a molecular dynamics simulation data.

3. Research Results and Achievements

3.1 HIVE and SURFACE

HIVE is an acronym standing for Heterogeneously Integrated Visual-Analytic Environment, which means that the system can be operated on computer systems with heterogeneous hardware architectures and multi-platform software systems. Figure 2 illustrates some of the appearances of the Web-based user interface of the HIVE system. The software architecture adopted by the HIVE is the server-client model thus it enables the users to operate the HIVE system even from their laptop computers. Figure 3 describes the software stack of the HIVE system.



(a) Workspace for visualization workflow design. (b) Viewing window and control area .

Figure 2. HIVE Web-based user interface.

SURFACE is an acronym standing for Scalable and Ubiquitous Rendering Framework for Advanced Computing Environments, and provides the necessary parallel rendering features to the HIVE system. SURFACE employs the ray tracing method, which is able to generate high-quality images, and is especially suitable for large-scale parallel processing.

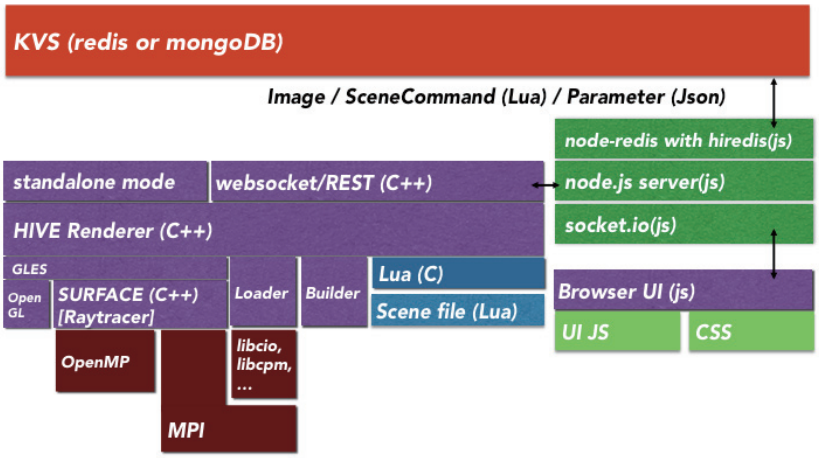


Figure 3. Software stack of the HIVE system.

3.2 Image Compositing

Parallel image compositing corresponds to the last stage of sort-last visualization approach where the parallel rendered images are combined into a single final image. In this year, we worked on an approach to convert non-power-of-two into power-of-two number of compositing nodes in order to enable the use of efficient image compositing algorithms for power-of-two number of nodes. In addition, we worked on an approach to execute large-scale image compositing in multiple steps in order to achieve better scalability.

Efficient parallel image compositing algorithms are worked by exchanging portions of the data, and combining them using appropriate image data merging techniques. It is well known that the exchanging and merging processes work well when the number of compositing nodes is power-of-two. Therefore, different approaches have been proposed to handle non-power-of-two number of compositing nodes. These approaches can be divided into single and multi-stage conversion. The single stage conversion, known as *Reduced* or *Folded* method, converts to the closest power of two ($m = 2^n$) smaller than the number of nodes ($m < m'$) by executing a reduction process known as *2-1 elimination*. We focused on the *2-3-4 Decomposition* approach, shown in Figure 4, for extending the reduction process including the *3-1* and *4-1 eliminations*. The main advantage of this approach is that the resulting number of nodes is smaller (2^{n-1}) compared to the *Reduced* method. This greatly helps to minimize the performance degradation when the number of compositing nodes becomes large. For instance, when the performance degradation between two consecutive power-of-two number of nodes (2^n and 2^{n+1}) is considerable, it becomes possible to achieve faster image compositing compared to the closest power-of-two number of nodes. That is, image compositing between $2^{n+1} + 1$ and $2^{n+2} - 1$ compositing nodes can be faster than using 2^{n+1}

compositing nodes since *2-3-4 Decomposition* reduces the number of compositing nodes to 2^n.

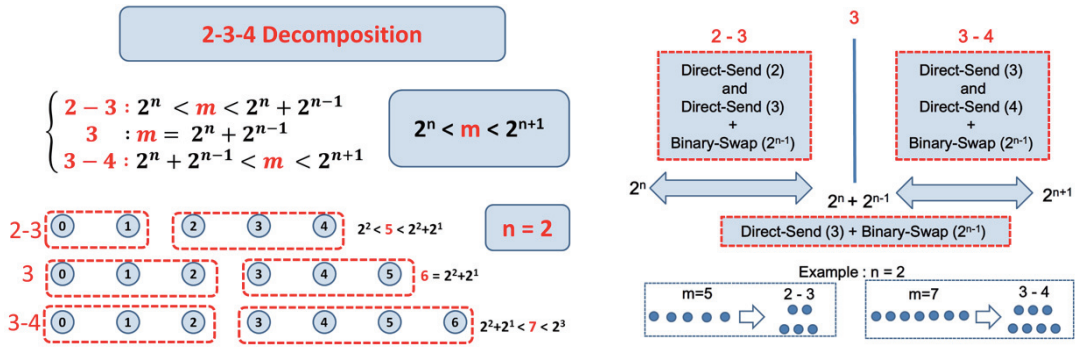


Figure 4. 2-3-4 Decomposition method with an example when n = 2 (Left), and its use in combination with different image compositing algorithms (Right).

Although *2-3-4 Decomposition* can minimize part of the performance degradation on large-scale parallel image compositing, it becomes inefficient when a massive number of compositing nodes in the range of tens of thousands are involved. In the case of K computer, it can reach 82,944 compositing nodes, in Hybrid MPI-OpenMP mode. Therefore, *2-3-4 Decomposition* can reduce it to 32,768 compositing nodes (2^{n-1}). It is worth to mention that the final image collecting is executed through *MPI_Gatherv* collective operation, and there exists a buffer overflow problem on the current MPI implementation for K computer, which does not allow the use of *MPI_Gatherv* with more than 50K nodes. Therefore, by reducing to the range of 32K compositing nodes, it becomes possible to avoid this problem. Although this considerable reduction, it is still in the range of tens of thousands of nodes where the performance degradation is prominent. In order to minimize this degradation, we focused on *Multi-Step* approach, shown in Figure 5, where the entire image compositing nodes are divided into smaller groups, with the size within the range where the performance is not greatly affected. By executing the full parallel image compositing at each of the groups, at the end it will produce partially composited images equal to the number of groups. We can recursively execute this group creation until the number of partially composited images becomes smaller than the group size. Since it only executes parallel image compositing using number of compositing nodes where the performance is not greatly affected, it will result in better scalability. Therefore, the aforementioned *2-3-4 Decomposition* will be greatly benefited.

```
m = Num_Global_Nodes
If ( m != Power-of-two )
  Do Reduction to Power-of-two

Nodes = Num_Nodes_Power of two
Rank = My_Rank_Power of two

While ( Nodes > Max. Group Size )
  Do
    Num_Groups = Nodes / Max. Group Size
    Create MPI Groups based on Rank
      Create MPI Communicator for these Groups
    Create MPI Groups for the Local Roots
      Create MPI Communicator for these Groups
    Nodes = Num_Groups
    Rank  =  New Rank inside the Group of Local Root
End Do
```

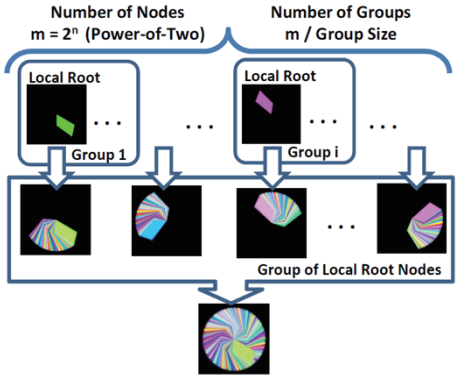


Figure 5. Multi-Step image compositing approach.

3.4 Compression of Large-Scale Dataset

M-Swap Method for Parallel POD Compression of Large-Scale Dataset.

In this paper, we presented a parallel data compression approach to reduce the size of time-varying big datasets. Firstly, we employ the proper orthogonal decomposition (POD) method for compression. The POD method can extract the underlying features of datasets to greatly reduce the size of big datasets. Meanwhile, the compressed datasets can be decompressed linearly. This feature can help scientists to interactively visualize big datasets for analysis. Then, we introduced a novel m-swap method to effectively parallelize the POD compression algorithm. The m-swap method can reach a high performance through fully using all parallel computing processors. In another word, no idle processors exist in the parallel compression process. Furthermore, the m-swap method can greatly reduce the cost of interprocessor communication. This is achieved by controlling the data transfer among $2m$ processors to obtain the best balance of computation cost of these processors.

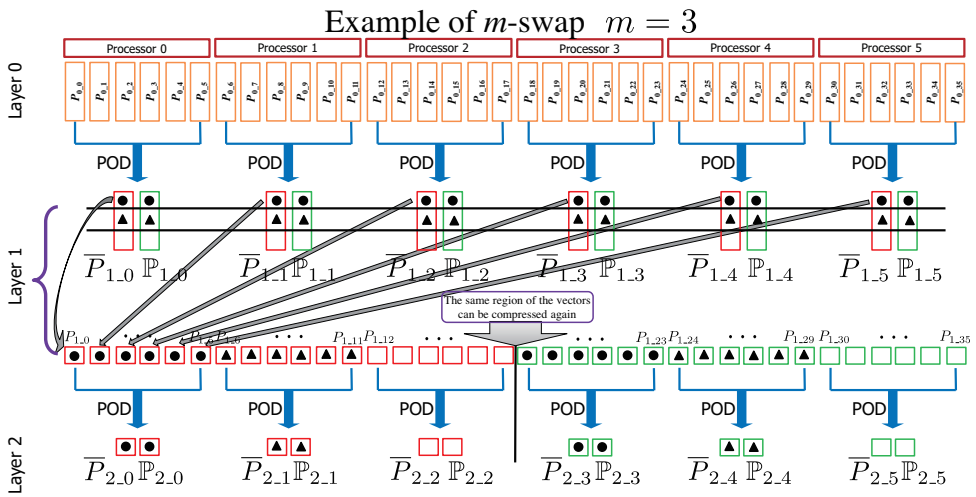


Figure 6. An example of parallel compressing a dataset with 36 time steps.

In our parallel framework, the compressed POD bases and POD mean vectors in different processors will be recursively compressed, respectively. The m-swap algorithm is designed to directly send and receive data among $2m$ (m >= 2) difference processors. Figure 6 shows an example of m = 3. Furthermore, unlike most existing parallel methods that can only deal with the datasets whose time steps number is power-of-two, the presented m-swap method can compress datasets with arbitrary time steps. Note that the binary swap (or 2-3 swap) method cannot be directly used for the POD compression method. Because the size of datasets does not change if two time steps are compressed into one POD mean vector and one POD basis.

Finally, the effectiveness of our m-swap method is demonstrated through compressing several big datasets on the K computer. Figure 7 is one of the results.

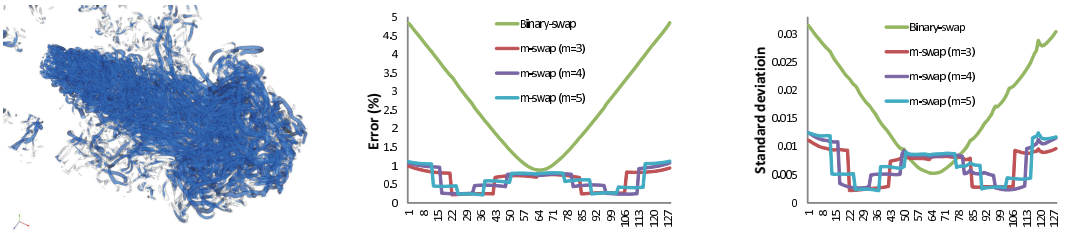


Figure 7. An example of compressing a dataset of the flow simulation in the air jet mixture of a machine. Its size if 300*200*200*128. The rendering result, the error, and the corresponding standard deviation of error are shown from left to right.

Fluid Data Compression and ROI Detection Using Run Length Method

Data compression and ROI (Region of Interest) detection are often used to improve efficiency of the visualization of numerical data. It is well known that the Run Length encoding is a good technique to compress the data where the same sequence appeared repeatedly, such as an image with little change, or a set of smooth fluid data. Another advantage of Run Length encoding is that it can be applied to every dimension of data separately. Therefore, the Run Length method can be implemented easily as a parallel processing algorithm. We proposed two different Run Length based methods. When using the Run Length method to compress a data set, its size may increase after the compression if the data does not contain many repeated parts. We only apply the compression for the case that the data can be compressed effectively. By checking the compression ratio, we can detect ROI. Figure 8 shows an example of compressing a 3D fluid data using Run Length method.

(X, Y, Z)	time direction		results of Run Length method
$(0, 0, 0)$	$[A\ A\ A\ \cdots\ A\ A]$	$\rightarrow$	$[A\ 257]$
$(1, 0, 0)$	$[A\ A\ A\ \cdots\ A\ A]$	$\rightarrow$	$[A\ 257]$
$(2, 0, 0)$	$[W\ A\ D\ \cdots\ A\ I]$	$\rightarrow$	$[W\ 1\ A\ 1\ D\ 1\ \cdots\ A\ 1\ I\ 1]$
$(3, 0, 0)$	$[A\ A\ A\ \cdots\ A\ A]$	$\rightarrow$	$[A\ 257]$
$(4, 0, 0)$	$[A\ A\ A\ \cdots\ A\ A]$	$\rightarrow$	$[A\ 257]$
$(5, 0, 0)$	$[A\ A\ A\ \cdots\ A\ A]$	$\rightarrow$	$[A\ 257]$
$(6, 0, 0)$	$[A\ A\ A\ \cdots\ A\ A]$	$\rightarrow$	$[A\ 257]$
$(7, 0, 0)$	$[A\ A\ A\ \cdots\ A\ A]$	$\rightarrow$	$[A\ 257]$
$(8, 0, 0)$	$[T\ H\ R\ \cdots\ E\ E]$	$\rightarrow$	$[T\ 1\ H\ 1\ R\ 1\ \cdots\ E\ 2]$
$\vdots$			
$(121, 361, 181)$	$[A\ A\ A\ \cdots\ A\ A]$	$\rightarrow$	$[A\ 257]$

Figure 8. An example of compressing a 3D fluid data using Run Length method.

4. Schedule and Future Plan

We will continuously improve our visualization framework by ameliorating the components of the software stack, and by aggregating new functionalities. We also have plans to give lectures regarding the visualization framework and its components.

5. Publication, Presentation and Deliverables

(1) Journal Papers

1. Shota Ishikawa, Haiyuan Wu, Chongke Bi, Qian Chen, Hirokazu Taki, and Kenji Ono, "Fluid Data Compression and ROI Detection Using Run Length Method," in Procedia Computer Science, Vol. 35, pp. 1284-1291, 2014.
2. Kenji Ono, Yasuhiro Kawashima, and Tomohiro Kawanabe, "Data Centric Framework for Large-scale High-performance Parallel Computation," Procedia Computer Science, Vol. 29, pp. 2336 – 2350, 2014.

(2) Conference Papers

1. Chongke Bi, Kenji Ono, Kwan-Liu Ma, Haiyuan Wu, and Toshiyuki Imamura, "Proper Orthogonal Decomposition Based Parallel Compression for Visualizing Big Data on the K Computer," in Proceedings of Eurographics Symposium on Parallel Graphics and Visualization, pp. 1-8, June, 2014.
2. Chongke Bi, Kenji Ono, and Lu Yang, "Parallel POD Compression of Time-Varying Big Datasets Using m-Swap on the K Computer," in Proceedings of IEEE International Congress on Big Data, pp. 438-445, June, 2014.
3. Hamed Khandan, "Introducing A-Cell for Scalable and Portable SIMD Programming,"

2014 IEEE 8th International Symposium on Embedded Multicore/Manycore SoCs (MCSoC), pp. 275-280, 2014.

4. Jorji Nonaka, Masahiro Fujita, and Kenji Ono, "Multi-Step Image Compositing for Massively Parallel Rendering," in Proceedings of the International Conference on High Performance Computing & Simulation 2014, Bologna, Italy, pp. 627-634, 2014.
5. Jorji Nonaka, Chongke Bi, Masahiro Fujita, and Kenji Ono, "2-3-4 Decomposition Method for Large-Scale Parallel Image Composition with Arbitrary Number of Nodes," in Proceedings of the First International Conference on Systems Informatics, Modelling and Simulation, Sheffield, UK, pp. 59-64, 2014.
6. Kenji Ono, Shuichi Chiba, Shunsuke Inoue, and Kazuo Minami, "Performance Improvement of Iterative Method with Bit-Representation technique for Coefficient Matrix," 11th International Meeting High Performance Computing for Computational Science, Eugene, Oregon, USA, June 30 - July 3, 2014.
7. Kenji Ono and Yasuhiro Kawashima and Tomohiro Kawanabe, "Data Centric Framework for Large-Scale High Performance Parallel Computation," International Conference on Computational Science, Cairns, Australia, June 10-12, 2014.
8. Hamed Khandan and Kenji Ono, "Knowledge Request-Broker Architecture: A Possible Foundation for a Resource-Constrained Dynamic and Autonomous Global System," 2014 IEEE World Forum on Internet of Things (WF-IoT), pp. 506-507, 2014.
9. Kenji Ono and Jorji Nonaka, "Active Subdomain Selection for Efficient Parallel Computation of Internal Flows in Complex Geometry," Books of extended abstracts of 26th International Conference on Computational Fluid Dynamics, pp. 112–113, 2014.

(3) Invited Talks

1. Kenji Ono, "Design of Practical Framework to utilize Big Data on Exascale Computer," ORAP Forum 33, CNRS, Paris, France, April, 2014.
2. Kenji Ono, "Scalable and Ubiquitous Visualization in Extreme-Scale Computational Environment," Extreme Performance Computational Science French-Japanese Conference, Embassy of France in Japan – Department for Science and Technology, Tokyo, Japan, April, 2014.

(4) Posters and presentations

1. Chongke Bi, "An m-Swap method for Parallel POD Compression on the K Computer," in Proceedings of Sparse Modeling High-Dimensional Data-Driven Science, pp. 165-166, December, 2014.
2. Chongke Bi, "In-situ Visualization of Big Data Using Sparse Modeling," in Proceedings of

Conference on Sparse Modeling, June, 2014.

3. Jorji Nonaka, Masahiro Fujita, Kenji Ono, Naohisa Sakamoto, Koji Koyamada, “A Study on Parallel PBVR for Large Data Visualization,” 第 42 回可視化情報シンポジウム, Tokyo, Japan, 2014.
4. Jorji Nonaka, Masahiro Fujita, Kenji Ono, “SURFACE: A Visualization Framework for Large-Scale Parallel Simulations,” Oral presentation at Ultrascale Visualization Workshop 2014, New Orleans-LA, USA, 2014.
5. Masahiro Fujita, Jorji Nonaka, and Kenji Ono, “LSGL: Large Scale Graphics Library for Peta-Scale Computing Environments,” Poster presentation at High Performance Graphics 2014, Lyon, France, 2014.
6. Kenji Ono, “CFD Applications for Industrial Design in Peta-Scale Computing Environments,” International HPC Summer School 2014, Budapest, Hungary, June 2-6, 2014.
7. Kenji Ono, “Bit-Representation of Boundary Conditions for High Performance Incompressible Thermal Flow Simulation,” 11th World Congress on Computational Mechanics (WCCM XI), Barcelona, Spain, July 20-25, 2014.
8. Shigueho Noda, Kazuyasu Sugiyama, Yasuhiro Kawashima, , Kenji Ono, Shu Takagi, , and Ryutaro Himeno, “Development and Applications of the Parallel Computing Middleware for the Life Science Simulations,” 11th World Congress on Computational Mechanics (WCCM XI), Barcelona, Spain, July 20-25, 2014.
9. Ken Uzawa, Kenji Ono, and Takanori Uchida, “Validation of Local SGS Models for High Reynolds Number Flow,” 11th World Congress on Computational Mechanics (WCCM XI), Barcelona, Spain, July 20-25, 2014.
10. Kenji Ono, “Challenges and Strategy to Tackle the Extreme-Scale Fluid Simulation for Engineering Process,” Japan/United States Exascale Applications Workshop, Gatlinburg, Tennessee, USA, September 5-6, 2014.
11. Jyunya Onishi, and Kenji Ono, “A Cartesian Grid Method for Simulating Two-Phase Flow in Complex Geometries,” 2nd International Conference on Numerical Methods in Multiphase Flows, Darmstadt, Germany, April, 2014.

(5) Patents and Deliverables

All released software products from this team are delivered via GitHub, and are available in the following repository: https://github.com/avr-aics-riken/

1. PMlib

   Performance Monitor library
2. SURFACE

Scalable and Ubiquitous Rendering Framework for Advanced Computing Environments

3. HIVE

   Heterogeneously Integrated Visualization Environment

4. CDMlib

   Cartesian Data Management library

5. PDMlib

   Particle Data Management library

6. JHPCN-DF

   Data compression library based on Jointed Hierarchical Precision Compression Number - Data Format

7. Text Parser

   Text Parser library that enables us to handle YAML-like simple text parameters

8. 234Compositor

   A parallel image composition library being developed to perform sort-last image composition on massively parallel environments.

Data Assimilation Research Team

1. Team members

Takemasa Miyoshi (Team Leader)
Shigenori Otsuka (Postdoctoral Researcher)
Koji Terasaki (Postdoctoral Researcher)
Keiichi Kondo (Postdoctoral Researcher)
Shunji Kotsuki (Postdoctoral Researcher)
Guo-Yuan Lien (Postdoctoral Researcher)
Yasumitsu Maejima (Research Associate)
Africa Perianez Santiago (Research Associate)
Hazuki Arakida (Technical Staff)
Gulanbaier Tuerhong (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)
Masaru Kunii (Visiting Scientist)
Kozo Okamoto (Visiting Scientist)
Michiko Otsuka (Visiting Scientist)
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 19 research and technical staff including 8 visiting members as of March 2015. Data assimilation is a cross-disciplinary science to synergize computer simulations and real-world 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 real-world data in the wisest way. Particularly, DA Team tackles challenging problems of developing efficient and accurate data assimilation systems for “big simulations” with real-world “big data” from various sources including advanced sensors. The specific foci include 1) theoretical and algorithmic developments for efficient

and accurate data assimilation, 2) data assimilation methods and applications by taking advantage of the world-leading K computer and "big data" from new advanced sensors, and 3) exploratory new applications of data assimilation in wider simulation fields. These advanced data assimilation studies will enhance simulation capabilities and lead to a better use of the K computer.

In FY2014, we continued on the ongoing 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 investigated (1 paper accepted).
2. The role of observation error correlations in data assimilation was investigated with the Lorenz-96 system (1 paper published).
3. Potential impact of assimilation order of observations in serial EnKF was investigated (1 paper under review).
4. Particle filter methods to treat non-Gaussian PDF were further explored.

[Leading research on meteorological applications]

5. Local Ensemble Transform Kalman Filter (LETKF) experiments with a large ensemble up to 10240 members were performed with both simulated and real cases, in collaboration with Large-scale Parallel Numerical Computing Technology Research Team (1 paper published, press release on July 23, 2014).
6. The LETKF system with the global Nonhydrostatic ICosahedral Atmospheric Model (NICAM) was improved and tested with the real conventional and satellite observations, in collaboration with Computational Climate Science Research Team (1 paper published).
7. Satellite-based global precipitation data were considered for assimilation with NICAM-LETKF (1 paper published).
8. "Big Data Assimilation" experiments for a selected case of local severe rainstorms in Kyoto on July 13, 2013, were performed to take advantage of Big Data from both high-resolution simulations and phased array weather radar data.
9. A new quality control algorithm for the Osaka phased array weather radar was developed (1 paper accepted).
10. The development of the LETKF system with the SCALE model was started in collaboration with Computational Climate Science Research Team.
11. Convective predictability was investigated by performing breeding experiments.
12. A precipitation nowcasting system was developed to take advantage of the dense and frequent

phased array weather radar data. The system was first explored by the three intern students, Ryota Kikuchi of Tohoku University, Yoshikazu Kitano of Hokkaido University, and Yusuke Taniguchi of University of Hyogo, supported by the AICS internship program.

13. Impact of dense and frequent ground observation data on local severe weather forecasting was investigated.

[Computational optimization]

14. The inter-node communication of the LETKF core module was enhanced for acceleration.

[Wider applications]

15. A particle filter was applied to a dynamical vegetation model known as the SEIB-DGVM (Spatially-Explicit, Individual-Based Dynamic Global Vegetation Model).

Three achievements are selected and highlighted in the next section.

3. Research Results and Achievements

3.1. 10240-member LETKF with the SPEEDY model (Miyoshi et al. 2014)

Data assimilation combines simulations and real-world data based on statistical mathematics, in which probability density function (PDF) plays an essential role. For example, the error correlations of the simulated state determine how the information of observations spreads in space and among different variables. Ensemble-based data assimilation employs usually up to 100 samples or ensemble simulations to represent the errors of the simulated state. However, it is known that small ensemble sizes cause a significant sampling error, so that the signal to noise ratio becomes problematic. Therefore, a number of techniques such as error covariance localization and inflation have been explored extensively in the field of ensemble-based data assimilation. Here, we take advantage of the world's leading K computer and performed a series of LETKF experiments with large ensembles up to 10240, largest ever for the global atmospheric circulation.

10240 is two orders of magnitude greater than the typical choices of up to 100, requiring 10^6 more computations for the eigenvalue decompositions in the LETKF. To accelerate the eigenvalue computations, we collaborated closely with Large-scale Parallel Numerical Computing Technology Research Team and implemented their EigenExa into our LETKF system. This successfully accelerated the computations by a factor of 8, and enabled 3-week computations of LETKF data assimilation cycles assimilating global conventional observations every 6 hours (i.e., 84 LETKF cycles). We performed simulated experiments using an atmospheric general circulation model (AGCM) with intermediate complexity, known as the SPEEDY model, which has a low resolution (30 horizontal wave numbers and 7 vertical levels) and simple physics schemes. We also started performing real-world experiments using the NICAM-LETKF system. Here, we focus the former (cf. RIKEN press release on July 23, 2014, http://www.riken.jp/en/pr/press/2014/20140723_2/).

Figure 1 illustrates 10240 simulated atmospheric states in a single picture to quickly glance at what

were computed. Here, we performed the LETKF data assimilation with simulated radiosonde (weather balloon) data. The 10240 atmospheric states are equally probable, and we find more similarities in the NH and differences in the SH, generally corresponding to the observing density. Radiosonde observations are made mainly over populated locations.

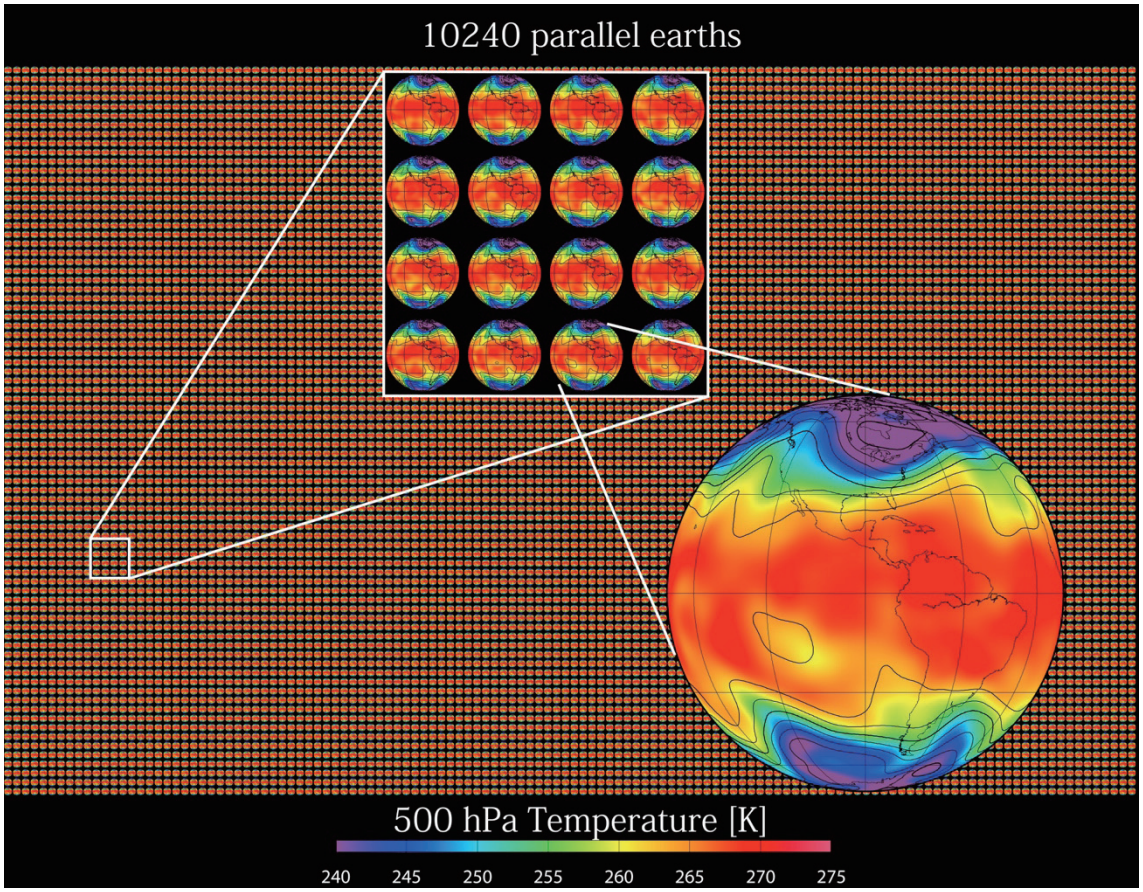


Figure 1. 10240 equally-probable global atmospheric states (temperature at the 500-hPa level).

Figure 2 left shows the spatial patterns of the error correlations for humidity from the yellow star point in the northern Pacific. We clearly find that the sampling errors are reduced significantly by increasing the ensemble size to 10240 from 100. Surprisingly, we find significant long-range error correlations extending in the planetary scales, so that the observation in the middle of Pacific may have significant impact in Siberia and even Eastern Europe. A possible future direction is to develop an efficient localization method that can capture such long-range correlations, and we may improve numerical weather prediction.

Figure 2 right shows the histogram of 100 and 10240 ensemble states of humidity at a single location. With 10240 samples or ensemble members, we find a clear bimodal structure, which is hardly captured by only 100 samples. We found that such strong non-Gaussianity occurred only

occasionally. We could think about future developments of more advanced data assimilation that considers non-Gaussianity adaptively only when and where necessary. The LETKF and most other data assimilation methods for large-scale problems are usually based on the Gaussian assumption.

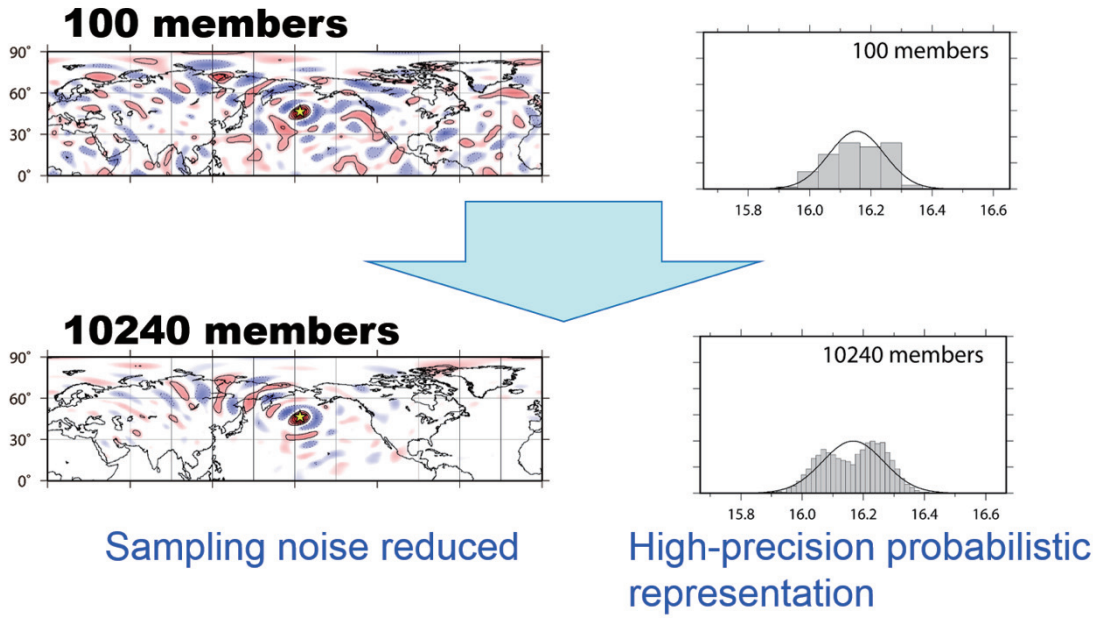


Figure 2. (Left) Spatial patterns of the error correlations for humidity from the yellow star point. This illustrates how the humidity observation at the star point makes the corrections in space. (Right) histograms of humidity (g kg^{-1}) at a single grid point.

3.2. Big Data Assimilation

With generous support by CREST, Japan Science and Technology Agency (JST), we have been working on the project titled "Innovating "Big Data Assimilation" technology for revolutionizing very-short-range severe weather prediction" (PI: Takemasa Miyoshi), or simply "Big Data Assimilation" (BDA) project, since October 2013. This project is a collaboration among RIKEN, Meteorological Research Institute, Meteorological Satellite Center, NICT (National Institute of Information and Communications Technology), and Osaka University, and almost 40 scientists are involved. DA Team plays a central role in this BDA project.

The main goal is to develop the BDA system that updates a 30-minute forecast at a 100-m resolution every 30 seconds by taking "big data" from new-generation sensors phased array weather radar (PAWR) and geostationary satellite Himawari-8 that produce orders of magnitude more data than the present counterparts. This way, we aim to resolve and capture precisely individual convective cells at a typical O(1)-km scale. The world's most advanced operational weather prediction systems update forecasts typically at an O(1)-km resolution every hour for convective-scale weather

forecasting. The BDA system is two orders of magnitude more rapid and an order of magnitude more precise.

A prototype system based on the JMA nonhydrostatic mesoscale model (NHM) was developed and tested in a single heavy rainfall case on July 13, 2013, when a series of severe convective rainstorms caused a disaster in Kyoto. Figure 3 shows the actual observations from the Osaka PAWR, showing that the convective cell does not change much in 30 seconds, but it changes significantly in 5 minutes. The conventional radar with a parabolic antenna needs to be rotated repeatedly at different elevation angles; it usually takes 5 minutes to scan 15 vertical scan angles. Figure 3 suggests that the data taken every 5 minutes may produce significant nonlinearity in the convective systems. By contrast, every-30-second data from PAWR seem to be frequent enough to make the linear and Gaussian assumptions that the current approaches of data assimilation in numerical weather prediction assume.

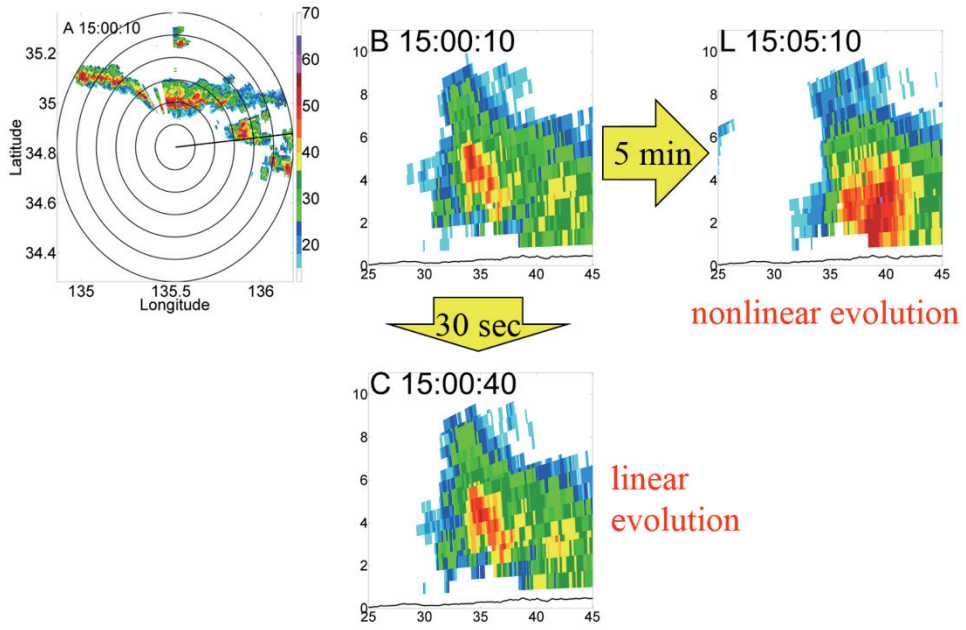


Figure 3. PAWR reflectivity (dBZ) on July 13, 2013. (Left) horizontal image at 15:00:10 JST, (Middle and Right) vertical cross sections along the line shown in the left panel at 15:00:10, 15:00:30, and 15:05:10 JST.

Our first trial of the case study was very promising. As shown in Fig. 4, the RMS errors dropped quickly in the first 4 minutes (8 data assimilation cycles), and the forecast was more accurate than the case without data assimilation for the entire 30-minute forecast period. We find that the individual convective cells matched the observations almost exactly due to “Big Data Assimilation” (Fig. 5).

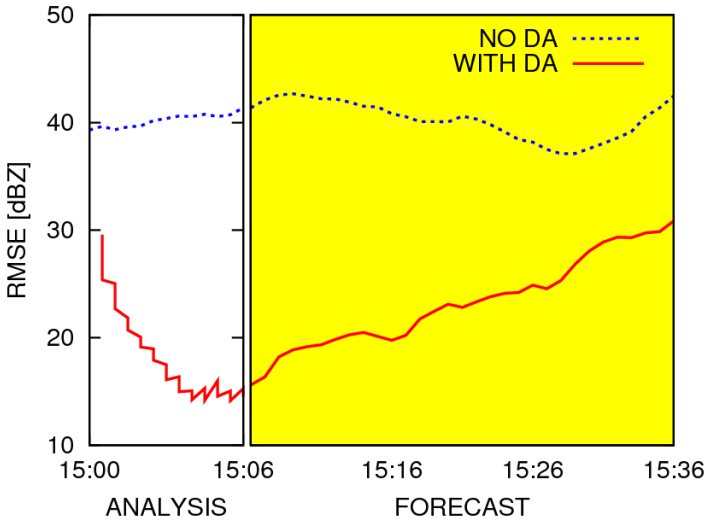


Figure 4. Time series of the rms errors relative to the observed reflectivity (dBZ). The observations were assimilated in the first 6 minutes (white background), and a 30-minute forecast was initialized at 15:06:00 JST (yellow background).

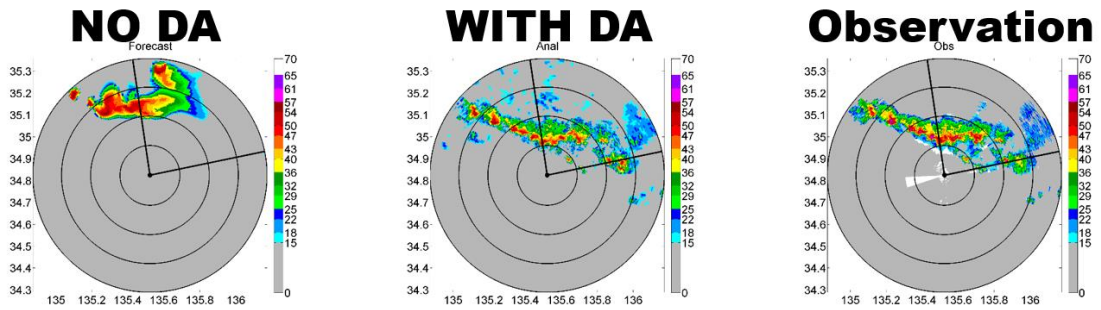


Figure 5. Horizontal maps of reflectivity (dBZ) at 15:06:00 JST.

3.3. New application to the dynamical vegetation model SEIB-DGVM

As one of the main foci of DA Team, we explore new applications of data assimilation. Since November 2013, we have been exploring data assimilation studies with the dynamical vegetation model SEIB-DGVM (Spatially-Explicit, Individual-Based Dynamic Global Vegetation Model). SEIB-DGVM simulates explicit individual plants (Fig. 6), so that the number of state variables, or the dimension of phase space, changes time to time as plants grow and die. It is not straightforward to perform Kalman-filter-based data assimilation in this type of dynamical system, so we decided to use a particle filter.

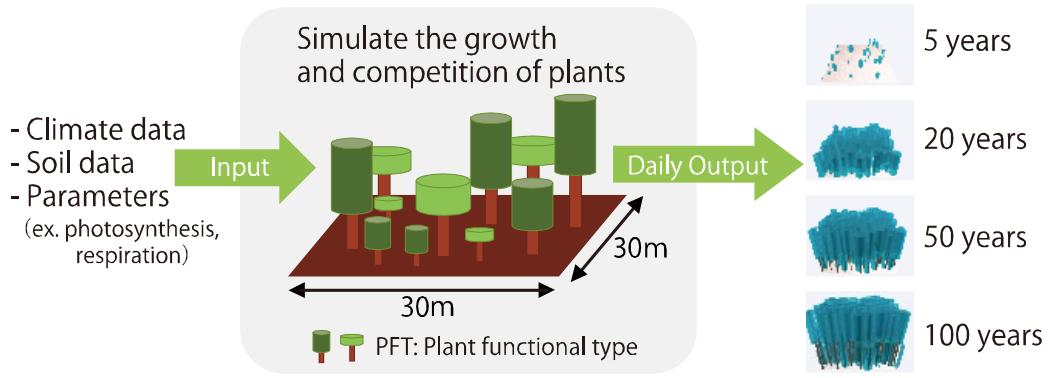


Figure 6. Schematic of vegetation simulation with SEIB-DGVM.

Figure 7 shows a schematic of the sequential importance resampling (SIR) particle filter. Particle filters consist of parallel simulations, a.k.a. particles, and each simulation or particle has probability. The probability is updated by taking observations. Observations have a likelihood function, and we use Bayes' theorem to update the probability: namely, the prior probability and likelihood function is multiplied and normalized to obtain the posterior probability for each particle. If we simply update the probability, some particles may have very small probability and add little value. To avoid performing useless simulations of little probability and to make the most use of limited computational resources, we omit the useless simulations and resample the states with larger probability. This way, the SIR filter normalizes the probability after resampling, so that every particle has equal probability. When resampling, we simply duplicate the high probability simulations, but with randomly perturbed to avoid exact duplication.

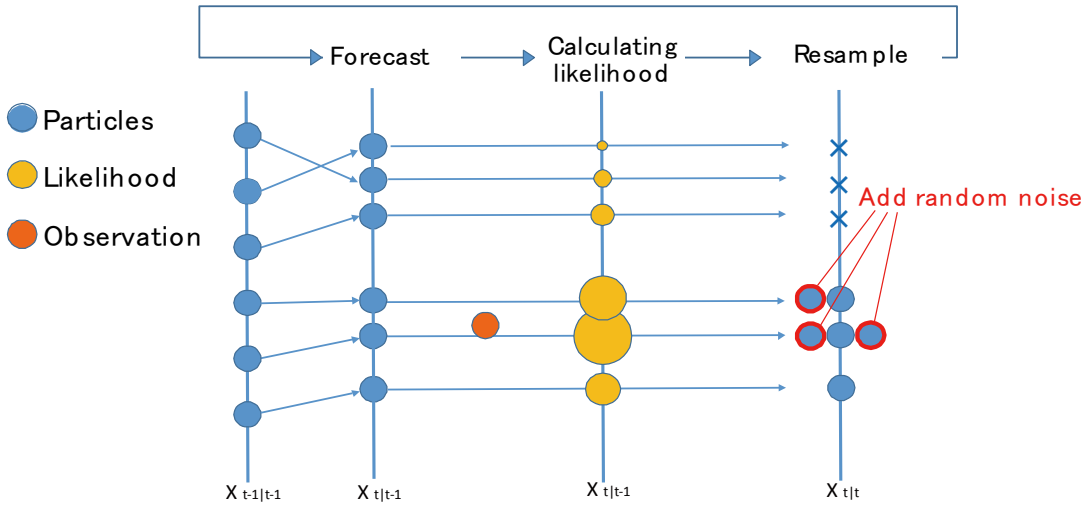


Figure 7. Schematic showing a sequential importance sampling (SIR) particle filter.

The SIR particle filter was applied to the SEIB-DGVM, and observing system simulation

experiments were performed. Here, we assumed LAI (leaf area index) observations from satellites. The LAI observations were simulated from the free nature run of the SEIB-DGVM. The nature run was generated by setting the three parameters of the SEIB-DGVM, maximum photosynthesis rate, foliate date, and dormant date, to be 36 μmolCO2 m^{-2} s^{-1}, 110th day of year, 210th day of year, respectively. The nature run was assumed to be the true states, and the true LAI values were perturbed randomly to simulate the satellite-based LAI observations. This way, we test if the SIR particle filter can estimate the state variables and model parameters by assimilating the LAI observations.

First, without data assimilation, we generated 800 parallel simulations or particles, the median and percentiles shown in Fig. 8 left. Figure 8 right panel shows 800 particles with data assimilation. We find that the SIR particle filter works very well with the SEIB-DGVM, so that the 800 particles become closer to the true states.

Figure 9 shows the parameter estimation results. These parameters were not observed directly, but estimated through data assimilation. The results indicate that the true parameter values are reasonably estimated by the SIR particle filter.

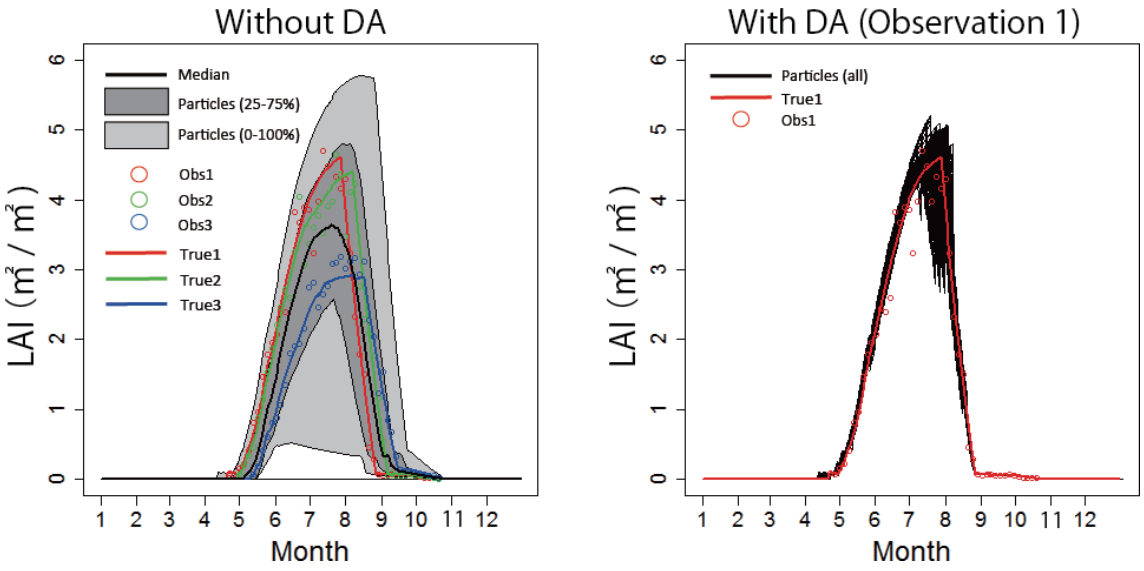


Figure 8. Time series of LAI, the observed variable. (Left) The true evolution is shown by red curve, and the observations are shown by red open circles. Ignore green and blue colors here. The black curve is the median of 800 particles without data assimilation, and grey shaded areas show the corresponding percentiles as shown in legend. (Right) Red curve and open circles are the same as the left panel, showing the nature run and observations, respectively. 800 particles with data assimilation are explicitly drawn.

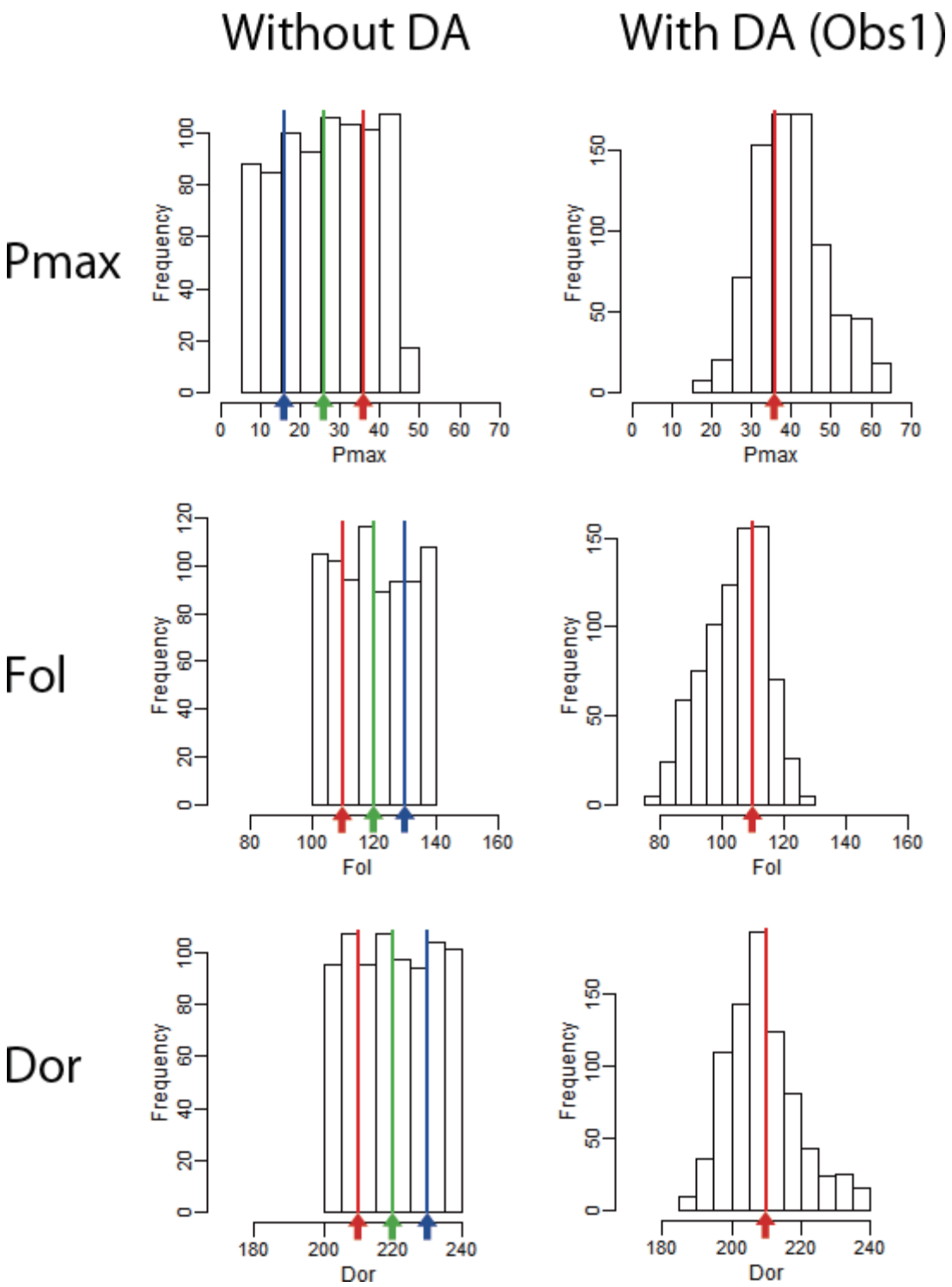


Figure 9. Parameter estimation results. Pmax, Fol, and Dor represent maximum photosynthesis rate (μmolCO2 m^{-2} s^{-1}), foliate date (day of year), and dormant date (day of year), respectively. Red bars indicate the true parameter values. White boxes indicate histograms of 800 particles: (Left) without data assimilation, (Right) with data assimilation.

4. Schedule and Future Plan

In FY2014, DA Team had four additional full-time research and technical staff and accepted more visiting researchers, leading to a continuing substantial growth. We continued our ongoing efforts on a wide range of data assimilation research on theoretical explorations, leading meteorological applications, algorithmic optimization, and wider applications. Our active research efforts have been making substantial impact on the scientific communities, and we are in a good shape in making progress on the research items of the AICS road-map. On February 23-26, we organized the fourth International Symposium on Data Assimilation (ISDA) 2015 at AICS. This event was received very well and attracted total 116 participants (42 from overseas and 16 from RIKEN), implying the successful development of DA research at AICS.

In FY2015, we will further extend and strengthen what we have achieved so far, and also will keep seeking new challenges. 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 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. 牛山朋來，佐山敬洋，岩見洋一，**三好建正**，2014：2011 年台風 12 号・15 号を対象としたアンサンブル降雨流出予測実験．河川技術論文集, 20, 455-460.
2. Cecelski, S. F., D.-L. Zhang, and **T. Miyoshi**, 2014: Genesis of Hurricane Julia (2010) within an African Easterly Wave: Developing and Non-Developing Members from WRF-LETKF Ensemble Forecasts. J. Atmos. Sci., 71, 2763-2781. doi:10.1175/JAS-D-13-0187.1
3. Tsai, C.-C., **S.-C. Yang**, and Y.-C. Liou, 2014: Improving Short-Term QPFs with a WRF-LETKF Radar Data assimilation system: OSSEs on Typhoon Morakot (2009). Tellus A, 66, 21804. doi:10.3402/tellusa.v66.21804
4. Huang, Z.-K., Z. Peng, H.-N. Liu, M.-G. Zhang, X.-G. Ma, **S.-C. Yang**, S.-D. Lee, and S.-Y. Kim, 2014: Development of CMAQ for East Asia CO2 data assimilation under an EnKF framework: a first result. Chinese Science Bulletin. doi:10.1007/s11434-014-0348-9.
5. Yoden, S., K. Ishioka, D. Durran, T. Enomoto, Y. Hayashi, **T. Miyoshi**, and M. Yamada, 2014: Theoretical Aspects of Variability and Predictability in Weather and Climate Systems. Bull. Amer. Meteor. Soc., 95, 1101-1104. doi:10.1175/BAMS-D-14-00009.1
6. Matsuoka, S., H. Sato, O. Tatebe, F. Takatsu, M. A. Jabri, M. Koibuchi, I. Fujiwara, S. Suzuki, M. Kakuta, T. Ishida, Y. Akiyama, T. Suzumura, K. Ueno, H. Kanezashi, and **T. Miyoshi**, 2014: Extreme Big Data (EBD): Next Generation Big Data Infrastructure

Technologies Towards Yottabyte/Year. Supercomputing Frontiers and Innovations, 1, No.2, 89-107. doi:10.14529/jsfi140206

7. Yoshimura, K., **T. Miyoshi**, and M. Kanamitsu, 2014: Observation System Simulation Experiments Using Water Vapor Isotope Information. J. Geophys. Res., 119. doi:10.1002/2014JD021662.
8. **Miyoshi, T.**, **K. Kondo**, and T. Imamura, 2014: The 10240-member ensemble Kalman filtering with an intermediate AGCM. Geophys. Res. Lett., 41. doi:10.1002/2014GL060863.
9. **Otsuka, S.**, M. Takeshita, and S. Yoden, 2014: A numerical experiment on the formation of the tropopause inversion layer associated with an explosive cyclogenesis: Possible role of gravity waves. Progress in Earth and Planetary Science, 1, 19. doi:10.1186/s40645-014-0019-0
10. Satoh, M., H. Tomita, H. Yashiro, H. Miura, C. Kodama, T. Seiki, A. Noda, Y. Yamada, D. Goto, M. Sawada, **T. Miyoshi**, Y. Niwa, M. Hara, T. Ohno, S. Iga, T. Arakawa, T. Inoue, H. Kubokawa, 2014: The non-hydrostatic icosahedral atmospheric model: description and development. Progress in Earth and Planetary Science, 1:18. doi:10.1186/s40645-014-0018-1.
11. **Kotsuki, S.**, **K. Terasaki**, and **T. Miyoshi**, 2014: GPM/DPR Precipitation Compared with a 3.5-km-resolution NICAM Simulation. SOLA, Vol: 10, pp.204-209. doi:10.2151/sola.2014-043
12. **Terasaki, K.**, and **T. Miyoshi**, 2014: Data Assimilation with Error-Correlated and Non-Orthogonal Observations: Experiments with the Lorenz-96 Model, SOLA, 10, 210-213. doi:10.2151/sola.2014-044.
13. **Yang, S.-C.**, S.-Y. Chen, S.-H. Chen, C.-Y. Huang and C.-S. Chen, 2013: Evaluating the impact of the COSMIC-RO bending angle data on predicting the heavy precipitation episode on 16 June 2008 during SoWMEX-IOP8. Mon. Wea. Rev., 142, 4139–4163. doi:10.1175/MWR-D-13-00275.1
14. **Terasaki, K.**, M. Sawada, and **T. Miyoshi**, 2015: Local Ensemble Transform Kalman Filter Experiments with the Nonhydrostatic Icosahedral Atmospheric Model NICAM. SOLA, 11, 23-26. doi:10.2151/sola.2015-006
15. Chang, C.-C., **S.-C. Yang** and C. Keppenne, 2014: Applications of the mean re-recentering scheme to improve typhoon track prediction: A case study of typhoon Nanmadol (2011), JMSJ Ser. II Vol. 92 (2014) No. 6 p. 559-584. doi:10.2151/jmsj.2014-604
16. Sawada, M., T. Sakai, T. Iwasaki, H. Seko, K. Saito and **T. Miyoshi**, 2015: Assimilating high-resolution winds from a Doppler lidar using an ensemble Kalman filter with lateral boundary adjustment. Tellus, 67A, 23473. doi:10.3402/tellusa.v67.23473

(2) Conference Papers

1. **島伸一郎**, “雲の物理学入門”, 物性研究 3, 033210 (2014). http://bussei-kenkyu.jp/pdf/03/3/9999-033210.pdf
2. **荒木田葉月**, 立澤史郎, 2014: 北極環境研究の長期構想 6 章「生物多様性を中心とする環境変化を解き明かす」:テーマ 8「陸域生態系と生物多様性への影響」- Q3「北極陸域生態系の変化が動物や気候に与える影響はどうなるか？」. 北極環境研究コンソーシアム(JCAR), p95-96.
   http://www.jcar.org/documents/longterm20140918_06_01.pdf
3. 立澤史郎, **荒木田葉月**, 2014: 北極環境研究の長期構想 5 章「現在進行中の地球温暖化に伴う北極の急激な環境変化を解き明かす」: テーマ 7「北極環境変化の社会への影響」- Q2「地球温暖化に起因する陸域環境の変化による影響は？」- b. 植生変化・野生動物・家畜 」. 北極環境研究コンソーシアム(JCAR), p83.
   http://www.jcar.org/documents/longterm20140918_05_07.pdf

(3) Invited Talks

1. **Shima**, S., “Preliminary numerical study on the cumulus-stratus transition induced by the increase of formation rate of aerosols”, Workshop on Space Climate, Solar Terrestrial Environment Laboratory, Nagoya University, Japan, 3rd April 2014
2. **Terasaki, K**. and **T. Miyoshi**, “Data assimilations with correlated observation errors and non-orthogonal observation operator”, ESA-DA workshop on correlated errors in data assimilation, University of Reading, Reading, UK, 24th April 2014.
3. **Miyoshi, T.**, “Recent activities on 'Big Data Assimilation' in Japan”, The 6th EnKF Workshop, Buffalo, NY, USA, 21st May 2014.
4. **Miyoshi, T**., "Numerical Weather Prediction and 'Big Data Assimilation'", International HPC Summer School 2014, Budapest, Hungary, 3rd June 2014.
5. **三好建正**, 別所康太郎, 瀬古弘, 富田浩文, 佐藤晋介, 牛尾知雄, 石川裕, “「ビッグデータ同化」によるゲリラ豪雨予測に向けて”, 画像電子学会年次大会, 東京, 2014 年 6 月 30 日
6. **Miyoshi, T.**, “‘Big Data Assimilation’ for Revolutionizing Weather Prediction”, the 53rd IDC HPC User Forum, Kobe, Japan, 16th July 2014.
7. **三好建正**, **“**DPR 降水量プロダクトと NICAM3.5km シミュレーションの比較”, DPR Quick Evaluation Team(QET)会合, 東京, 2014 年 7 月 24 日
8. **Miyoshi, T.**, **M. Kunii**, **J. Ruiz**, H. Seko, S. Satoh, T. Ushio, Y. Ishikawa, H. Tomita, K. Bessho, Session SCI-PS137, “Recent activities on “Big Data Assimilation” in Japan”, WWOSC 2014, Montreal, Canada, 17th August 2014.
9. **三好建正**, “ビッグデータ同化”, 東京大学大気海洋研究所 国際沿岸海洋研究セン

ター　共同利用研究集会　中緯度気象・気候研究の現状と展望, 大槌, 岩手, 2014 年 8 月 27 日.

10. **三好建正**, “ビッグデータ時代のデータ同化”, グリッド協議会神戸セミナー, 神戸, 2014 年 9 月 12 日.
11. **島伸一郎**, “次世代エクサ級スパコンによるゲリラ豪雨予測に向けた気象モデルの開発”, 兵庫県立大学知の交流シンポジウム 2014, 2014 年 9 月 24 日
12. **Miyoshi, T.**, “Big Data Assimilation” revolutionizing severe weather forecasting, Joint Workshop of 6th International Workshop on Global Cloud Resolving Modeling and 3rd International Workshop on Nonhydrostatic Numerical Models, Kobe, Japan, 25th September 2014.
13. **Miyoshi, T.**, “‘Big Data Assimilation’ revolutionizing severe weather forecasting”, Workshop on perspectives in computational climate science and 7th OFES International Workshop, Aizu-wakamatsu, Japan, 2nd October 2014.
14. **Miyoshi, T.**, “‘Big Data Assimilation’ Revolutionizing Weather Prediction”, 13th Japan Science and Technology Agency (JST) Advisory Committee Meeting, Kyoto, Japan, 3rd October 2014.
15. **三好建正**, “「ビッグデータ同化」でゲリラ豪雨に挑む”, パターン認識・メディア理解（PRMU）研究会, 幕張, 2014 年 10 月 9 日.
16. **三好建正**, “データ同化の今後の展望”, 日本気象学会 地球観測衛星研究連絡会, 福岡, Japan, 2014 年 10 月 23 日.
17. **三好建正**, “「ビッグデータ同化」でゲリラ豪雨に挑む”, 第 37 回情報化学討論会, 豊橋, 2014 年 11 月 28 日.
18. **三好建正**, “ビッグデータ時代のデータ同化”, 第 14 回 PC クラスタシンポジウム, 2014 年 12 月 12 日
19. **Miyoshi, T.**, “‘Big Data Assimilation’ Revolutionizing Severe Weather Forecasting”, the 95th AMS Annual Meeting, American Meteorological Society, 19th Conference on Integrated Observing and Assimilation Systems for Atmosphere, Oceans, and Land Surface (IOAS-AOLS), Phoenix, AZ, USA, 5th January 2015.
20. **三好建正**, “Ensemble-based Data Assimilation of TRMM/GPM Precipitation Measurements”, PMM PI ワークショップ, 東京, 2015 年 1 月 15 日
21. **三好建正**, “データ同化の応用に向けた展望”, 第 7 回 EFD/CFD 融合ワークショップ, 東京, 2015 年 1 月 26 日
22. **Miyoshi, T.**, “‘Big Data Assimilation’ Revolutionizing Severe Weather Forecasting”, the 4th International Symposium on Data Assimilation, Kobe, 23rd February 2015.
23. **三好建正**, **小槻峻司**, **寺崎康児**、**Guo-Yuan Lien**, 富田浩文, 佐藤正樹, Eugenia Kalnay, “衛星降水観測データの全球大気モデル NICAM への同化に向け

て", GSMaP 及び衛星シミュレータ研究集会, 名古屋, 2015 年 3 月 2 日.

24. **島伸一郎**, "動的植生モデル SEIB-DGVM を用いたデータ同化実験, 他", 香川非線形研究会, 香川大学, 2015 年 3 月 3-4 日.
25. **Shima**, S., "Numerical study on the cumulus-stratus transition using the super-droplet method", International Workshop on Cloud Turbulence, Nagoya Institute of Technology, Nagoya, Japan, 4th-6th March 2015.

(4) Posters and presentations

1. **Kunii, M.**, "Data assimilation experiments for TCs with the LETKF", Japan Geoscience Union Meeting 2014, Yokohama, 29th April 2014.
2. 渡邊歩佳, 今村 剛, **前島康光**, "火星における対流励起重力波と熱圏への影響", 日本地球惑星科学連合 2014 年大会, 横浜, 2014 年 5 月 1 日
3. **Kotsuki, S.**, **T. Miyoshi**, and S. Greybush, "Does the assimilation order matter in the serial ensemble Kalman filter? A study with the Lorenz-96 model", the 6th EnKF Workshop, Buffalo, NY, USA, 19th May 2014.
4. **Kondo, K.** and **T. Miyoshi**, "The dual-localization approach and large ensemble data assimilation in the SPEEDY-LETKF", the 6th EnKF Workshop, Buffalo, New York, 19th May 2014.
5. **Otsuka, S.** and **T. Miyoshi**, "A Bayesian optimization approach to multi-model ensemble Kalman filter", the 6th EnKF Workshop, Buffalo, NY, USA, 19th May 2014.
6. **Terasaki, K.**, M. Sawada and **T. Miyoshi**, "Developing the Local Ensemble Transform Kalman Filter with the Japanese Icosahedral Global Model NICAM", the 6th EnKF Workshop, Buffalo, NY, USA, 21th May 2014.
7. **前島康光**, 橋本明弘, 村上正隆, 池田明弘, 伊東克郎, 水野克彦, 松尾崇宏, Richard D. Farley, "小河内ダム集水域におけるシーディングシミュレーション(その 2)", 日本気象学会 2014 年度春季大会, 横浜, 2014 年 5 月 23 日
8. 渡邊歩佳, 今村 剛, **前島康光, "**火星における対流励起重力波と熱圏への影響", 気象学会 2014 年度春季大会, 横浜, 2014 年 5 月 23 日
9. 今村 剛, 樋口武人, **前島康光,** 高木征弘, 杉本憲彦, 池田恒平, 安藤紘基, "金星雲層における日射による対流の抑制", 気象学会 2014 年度春季大会, 横浜, 2014 年 5 月 24 日
10. **Kunii, M.**, "Data assimilation experiments of TC position and intensity with an ensemble Kalman filter", 2014 Meteorological Society of Japan Spring Meeting, Yokohama, 24th May 2014.
11. **小槻峻司, "**画像の類似性判定、統計的仮説検定、on-off インターミッテンシー", 第 3 回 理研・京大合同データ同化研究会, 神戸, 2014 年 7 月 28 日

12. **近藤圭一, 三好建正,** "10240 メンバーSPEEDY-LETKF を用いた PDF 解析", 第 3 回 理研・京大合同データ同化研究会, 神戸, 2014 年 7 月 28 日
13. **Lien, G.-Y.**, E. Kalnay, and **T. Miyoshi**, "Ensemble assimilation of global large-scale precipitation", AOGS 11th Annual Meeting, Sapporo, Japan, 28th Jul-1st Aug 2014.
14. **Otsuka, S.**, M. Takeshita, and S. Yoden, "Diagnosis on gravity waves and their role in extratropical tropopause inversion layers simulated by a regional model", AOGS2014, Sapporo, 30th July 2014.
15. Alicia, P. K. Tanaka K, **S. Kotsuki**, and S. Tanaka, "Reproduction of Past Surface Parameters and its Application to Regional Climate Change Study in Paraguay", AOGS2014, Sapporo, 31th July, 2014.
16. **Otsuka, S.** and **T. Miyoshi**, "A Bayesian Optimization of the Ensemble Sizes in Multi-model Ensemble Kalman Filter", AOGS2014, Sapporo, 31st July 2014.
17. Pierre Tandeo, Pierre Ailliot, Ronan Fablet, **Juan Ruiz**, François Rousseau and Bertrand Chapron, "The Analog Ensemble Kalman Filter and Smoother", the 4th international Workshop on Climate Informatics, 25th-26th September 2014.
18. Felix Carrasco, **Juan Ruiz**, Celeste Saulo, Axel Osses, "Experimenting with the LETKF in a dispersion model coupled with the Lorenz 96 model", WWOSC2014, Montreal, 16th-21st August 2014.
19. María Eugenia Dillon, Yanina García Skabar, **Juan Ruiz**, Eugenia Kalnay, Estela A. Collini, Pablo Echevarría, Marcos Saucedo and Takemasa Miyoshi, "Application of the WRF-LETKF system over Southern South America: Sensitivity to model physics", WWOSC2014, Montreal, 16th-21st August 2014.
20. **Juan Ruiz**, **Takemasa Miyoshi** and **Masaru Kunii**, "How do model error and localization approaches affect model parameter estimation in the LETKF?", WWOSC2014, Montreal, 16th-21st August 2014.
21. Marcos Saucedo, **Juan Ruiz** and Celeste Saulo, "Sensitivity experiments to design a regional assimilation system combining the LETKF and the WRF model", WWOSC2014, Montreal, 16-21 August 2014.
22. Tanaka K. and **S. Kotsuki**, "Projection of Future Change in Aridity Index and Evaporation Ratio in the Arid and Semi-Arid Region", the Second International Conference on Arid Land Studies, Samarkand, Uzbekistan, 9th September 2014.
23. **Shima, S.**, "Preliminary numerical study on the cumulus-stratus transition induced by the increase of formation rate of aerosol", the 6th GCRM and 3rd NHM WS, Kobe, Japan, 24th-26th September 2014.
24. **Otsuka, S.** and **T. Miyoshi**, "Convective-scale predictability in WRF simulations at a 100-m resolution", the 6th GCRM and 3rd NHM WS, Kobe, Japan, 24th-26th September

2014.

25. **小槻峻司**，田中賢治，樋口篤志，本間香貴，篠田太郎，相馬一義，竹中栄晶，可知美佐子，久保田拓志，梶原康司:, “環太平洋域を対象とした陸面再解析・速報解析システムの開発: －日本域における高解像度陸面再解析－”，水文・水資源学会 2014 年研究発表会，宮崎, 2014 年 9 月 25 日
26. 田中賢治, 峠嘉哉, 浅野倫矢, **小槻峻司，“**陸域水循環解析における気象強制力データの問題点”，水文・水資源学会 2014 年研究発表会，宮崎, 2014 年 9 月 27 日
27. **Kotsuki, S.**, **K. Terasaki** and **T. Miyoshi**, “Comparative study of GPM-derived precipitation with the 3.5-km-resolution NICAM simulations”, the 6th GCRM and 3rd NHM WS, Kobe, Japan, 24th-26th September 2014.
28. **Terasaki, K.**, “Developing the Local Ensemble Transform Kalman Filter with the Japanese Icosahedral Global Model NICAM”, the 6th GCRM and 3rd NHM WS, Kobe, Japan, 24th-26th September 2014.
29. **Maejima, Y.**, **M. Kunii**, H. Seko, K. Sato, R. Maeda and **T. Miyoshi**, “Impacts of dense and frequent surface observations on severe rainstorm forecasts”, the 6th GCRM and 3rd NHM WS, Kobe, Japan, 24th-26th September 2014.
30. **Kunii, M.**, **T. Miyoshi**, **J. Ruiz,** T. Ushio, S. Satoh, K. Bessho and H. Seko, “30-second-update ensemble Kalman filter experiments using JMA-NHM at a 100-m resolution”, the 6th GCRM and 3rd NHM WS, Kobe, Japan, 24th-26th September 2014.
31. Alicia, P., K. Tanaka, **S. Kotsuki**, and S. Tanaka, “Reproduction of Long-term Surface Parameters and its Application to Regional Climate Change Study in Paraguay”，水文・水資源学会 2014 年研究発表会，宮崎, 2014 年 9 月 27 日
32. **寺崎康児**, “NICAM-LETKF の開発状況”, NICAM 開発者会議, JAMSTEC 東京事務所, 2014 年 10 月 14 日
33. **国井勝**, **Juan Ruiz**, **Guo-Yuan Lien**，**三好建正**，牛尾知雄，佐藤晋介，瀬古弘，別所康太郎, “水平解像度 100m の NHM を用いた 30 秒サイクルデータ同化実験”，日本気象学会 2014 年度秋季大会，福岡, 2014 年 10 月 21 日.
34. **大塚成徳**，**三好建正，“**100m 解像度の領域モデルによる積雲対流のブリーディング実験”，日本気象学会 2014 年度秋季大会，福岡, 2014 年 10 月 21 日.
35. **前島康光**，**國井勝，**瀬古弘，前田亮太，佐藤香絵，**三好建正，“**2008 年 7 月 28 日に神戸市付近で発生した局地的大雨の 観測システムシミュレーション実験”，日本気象学会 2014 年度秋季大会，福岡, 2014 年 10 月 21 日.
36. **近藤圭一**，**三好建正，“**10240 メンバーによるアンサンブルデータ同化実験”，日本気象学会 2014 年度秋季大会，福岡, 2014 年 10 月 22 日
37. **大塚道子**，**国井勝，**瀬古弘，下地和希，林昌弘，今井崇人, “MTSAT-1R によるラピッドスキャンデータのメソスケールデータ同化への利用”，気象学会 2014 年度秋季

大会, 福岡, 2014 年 10 月 22 日.

38. **寺崎康児**, 沢田雅洋, **三好建正,** "全球非静力学モデル NICAM を使った 局所アンサンブルカルマンフィルタ LETKF", 日本気象学会 2014 年度秋季大会, 福岡, 2014 年 10 月 22 日.
39. **小槻峻司, 寺崎康児, 三好建正,** "GPM/DPR 地上降水量データの初期検証：3.5km NICAM との比較", 気象学会 2014 年度秋季大会, 福岡, 2014 年 10 月 23 日.
40. Higuchi, A., H. Takenaka, H. Hirose, M.K. Yamamoto, **S. Kotsuki**, H. Irie, K. Tanaka and M. Hayasaki, "CEReS archived satellites related datasets and these applications", the 22nd CEReS International Symposium, Yogyakarta, Indonesia, 29th October 2014.
41. **島伸一郎**, "不変多様体を使った連結階層シミュレーションの試み", 第 1 回計算科学連携センター学術会議, 兵庫県立大学, 2014 年 11 月 5 日.
42. **前島康光**, **國井勝,** 瀬古弘, 前田亮太, 佐藤香絵, **三好建正,** "2008 年 7 月 28 日に神戸市付近で発生した局地的大雨の 観測システムシミュレーション実験", 急発達する低気圧の実態・予測・災害軽減に関する研究集会, 京都, 2014 年 11 月 17 日
43. **大塚成徳**, **三好建正,** "100ｍ解像度の領域モデルによる積雲対流のブリーディング実験", 急発達する低気圧の実態・予測・災害軽減に関する研究集会, 宇治, 2014 年 11 月 17 日.
44. **寺崎康児**, 沢田 雅洋, **三好建正,** "NICAM-LETKF システムの開発と現状", 急発達する低気圧の実態・予測・災害軽減に関する研究集会, 宇治, 2014 年 11 月 17 日
45. **近藤圭一, 三好建正,** "10240 メンバーを用いたアンサンブルデータ同化実験", 急発達する低気圧の実態・予測・災害軽減に関する研究集会, 宇治, 2014 年 11 月 17 日
46. **Kotsuki, S.**, **K. Terasaki** and **T. Miyoshi**, "Comparative study of GPM-derived precipitation with the 3.5-km-resolution NICAM simulations", 7th IPWG Workshop on Precipitation Measurements, Tsukuba, Japan, 17th-21st November 2014.
47. **Shima**, S., "Data assimilation experiments of the dynamic global vegetation model SEIB-DGVM with simulated GPP observations", Data Assimilation Seminar, RIKEN-AICS, 26th November 2014.
48. **Kotsuki, S.**, **K. Terasaki** and **T. Miyoshi**, "Comparative study of GPM-derived precipitation with the 3.5-km-resolution NICAM simulations", the 5th AICS International Symposium, Kobe, Japan, 8th-9th December 2014.
49. **Kunii, M.**, **J. Ruiz**, **G. Lien**, T. Ushio, S. Satoh, K. Bessho, H. Seko and **T. Miyoshi**, "30-second-update ensemble Kalman filter experiments using JMA-NHM at a 100-m resolution", the 5th AICS International Symposium, Kobe, Japan, 8th-9th December 2014.
50. **Terasaki, T.**, M., Sawada, and **T., Miyoshi**, "Local Ensemble Transform Kalman Filter

Experiments with the Nonhydrostatic Icosahedral Atmospheric Model NICAM", the 5th AICS International Symposium, Kobe, Japan, 8th-10th December 2014.

51. **Lien, G.-Y.**, **T. Miyoshi**, S. Nishizawa, H. Yashiro, R. Yoshida, and H. Tomita, "Ensemble data assimilation for a large parallel numerical weather prediction model: Development of the SCALE-LETKF system", the 5th AICS International Symposium, Kobe, Japan, 8th-9th December 2014.
52. **G. Tuerhong**, **S. Otsuka**, **J. Ruiz**, R. Kikuchi, Y. Kitano, Y. Taniguchi, and **T. Miyoshi**, "Short term forecasting for precipitation by utilizing a new three-dimensional super-rapid phased array weather radar data", the 5th AICS International Symposium, Kobe, Japan, 8th-9th December 2014.
53. **Maejima, Y.**, **M. Kunii**, H. Seko, K. Sato, R. Maeda and **T. Miyoshi**, "Toward investigating the impacts of dense and frequent surface observations on severe rainstorm forecasts", the 5th AICS International Symposium, Kobe, 8th-9th December 2014.
54. **Otsuka, S.** and **T. Miyoshi**, "Convective-scale predictability in numerical weather prediction at a 100-m resolution", the 5th AICS International Symposium, Kobe, 8th-9th December 2014.
55. **Kondo, K.**, and **T., Miyoshi**, "The 10,240-member ensemble Kalman filtering with an intermediate AGCM without localization", the 5th AICS International Symposium, Kobe, Japan, 8th-9th, December 2014.
56. **Arakida, H.**, **T. Miyoshi**, T. Ise, **S. Shima**, "Data assimilation experiments with simulated LAI observations and the dynamic global vegetation model SEIB-DGVM", the 5th AICS International Symposium, Kobe, 8th-9th December 2014.
57. **Kotsuki, S.**, **K. Terasaki** and **T. Miyoshi**, "Comparative study of GPM-derived precipitation with the 3.5-km-resolution NICAM simulations", AGU Fall Meeting, San Francisco, USA, 15th-19th December 2014.
58. **Miyoshi, T.**, **S. Kotsuki**, **K. Terasaki**, **G. Y. Lien**, and E. Kalnay, "Toward Assimilation of GPM-derived Precipitation Data with NICAM-LETKF", Eugenia Kalnay Symposium, AMS Annual Meeting, Phoenix, AZ, USA, 6th January 2015.
59. **Miyoshi, T.**, **K. Terasaki**, M. Sawada, and **S. Kotsuki**, "Local Ensemble Transform Kalman Filter with Nonhydrostatic Icosahedral Atmospheric Model NICAM", IOAS-AOLS, AMS Annual Meeting, Phoenix, AZ, USA, 6th January 2015.
60. **Kondo, K.**, and **T., Miyoshi**, "The 10,240-member ensemble Kalman filtering with an intermediate AGCM without localization", 95th AMS annual meeting, Phoenix, USA, 4th-8th January 2015.
61. **Lien, G.-Y.**, E. Kalnay, D. Hotta, and **T. Miyoshi**, "Ensemble forecast sensitivity to the observations (EFSO) applied to precipitation data assimilation", the 4th International

Symposium on Data Assimilation, Kobe, Japan, 23rd-26th February 2015.

62. **S. Otsuka** and **T. Miyoshi**, "Convective-scale predictability in numerical weather prediction at a 100-m resolution", the 4th International Symposium on Data Assimilation, Kobe, Japan, 23rd-26th February 2015.
63. **S. Otsuka**, **G. Tuerhong**, **J. Ruiz**, R. Kikuchi, Y. Kitano, Y. Taniguchi, and **T. Miyoshi**, "Precipitation nowcasting with a new three-dimensional super-rapid phased array weather radar", the 4th International Symposium on Data Assimilation, Kobe, Japan, 23rd-26th February 2015.
64. **Kotsuki, S.**, **K., Terasaki**, and **T., Miyoshi**, "GPM/DPR precipitation compared with a 3.5-km-resolution NICAM simulation", the 4th International Symposium on Data Assimilation, Kobe, Japan, 23rd-26th February 2015.
65. **Arakida, H.**, **T. Miyoshi**, T. Ise, **S. Shima**, "Data assimilation experiments with simulated LAI observations and the dynamic global vegetation model SEIB-DGVM", the 4th International Symposium on Data Assimilation, Kobe, Japan, 23rd-26th February 2015.
66. **Lien, G.-Y.**, **T. Miyoshi**, S. Nishizawa, H. Yashiro, R. Yoshida, and H. Tomita, "Development of the SCALE-LETKF system for radar data assimilation", the 4th International Symposium on Data Assimilation, Kobe, Japan, 23rd-26th February 2015.
67. **Maejima, Y.**, **M. Kunii**, H. Seko, K. Sato, R. Maeda and **T. Miyoshi**, "Toward investigating the impacts of dense and frequent surface observations on severe rainstorm forecasts", the 4th International Symposium on Data Assimilation, Kobe, Japan, 23rd-26th February 2015.
68. **Kondo, K.**, and **T., Miyoshi**, "The 10,240-member ensemble Kalman filtering with an intermediate AGCM without localization", the 4th International Symposium on Data Assimilation, Kobe, Japan, 23rd-26th February 2015.
69. **Kotsuki, S.**, **K., Terasaki**, **G.-Y., Lien**, **T., Miyoshi**, and E., Kalnay, "Ensemble Data Assimilation of GSMaP precipitation into the nonhydrostatic global atmospheric model NICAM", the 4th International Symposium on Data Assimilation, Kobe, Japan, 23rd-26th February 2015.
70. **Terasaki, T.**, and **T., Miyoshi**, "Applying the four-dimensional Local Ensemble Transform Kalman Filter to the Nonhydrostatic Icosahedral Atmospheric Model NICAM", the 4th International Symposium on Data Assimilation, Kobe, Japan, 23rd-26th February 2015.
71. **Perianez, A.**, J. A. Otkin, A. Schomburg, R. Faulwetter, H. Reich, C. Schraff, R. Potthast, K. Okamoto, K. Bessyo, H. Seko and T. Miyoshi, "Cloud-affected Infrared Brightness Temperature Assimilation using a Local Ensemble Transform Kalman Filter", the 4th International Symposium on Data Assimilation, Kobe, Japan, 23rd-26th February 2015.
72. **Otsuka, M.**, **M. Kunii**, H. Seko, K. Shimoji, M. Hayashi, T. Imai, "Assimilation

experiments of MTSAT rapid scan data", the 4th International Symposium on Data Assimilation, Kobe, Japan, 23rd-26th February 2015.

73. **Masaru Kunii**, **Juan J. Ruiz**, **Guo-Yuan Lien**, Tomoo Ushio, Shinsuke Satoh, Kotaro Bessho, Hiromu Seko and **Takemasa Miyoshi**, "30-second-update ensemble Kalman filter experiments using JMA-NHM at a 100-m resolution", the 4th International Symposium on Data Assimilation, Kobe, Japan, 23rd-26th February 2015.
74. **Kotsuki, S.**, **K., Terasaki**, **G.-Y., Lien**, **T., Miyoshi**, and E., Kalnay, "Assimilating TRMM/GPM-derived Precipitation with NICAM-LETKF", the 5th DAWS, Kobe, Japan, 27th February 2015.
75. **Terasaki, T.**, and **T., Miyoshi**, "Applying the four-dimensional Local Ensemble Transform Kalman Filter to the Nonhydrostatic Icosahedral Atmospheric Model NICAM", the 5th DAWS, Kobe, Japan, 27th February 2015.
76. **小槻峻司，荒木田葉月，三好建正，**田中賢治, "水資源・作物結合モデルの開発とデータ同化への展望", 日本農業気象学会　2015 年全国大会, つくば, 2015 年 3 月 16-19 日.
77. **Arakida, H.**, **T. Miyoshi**, T. Ise, S. Shima, "Data assimilation experiments with simulated LAI observations and the dynamic global vegetation model SEIB-DGVM", Annual Meetings of Ecological Society of Japan, Kagoshima, 18th-22th March 2015.

(5) Patents and Deliverables

The LETKF code is updated as needed and available at https://code.google.com/p/miyoshi/.

(6) Awards

1. **三好建正**: 科学技術分野の文部科学大臣表彰　若手科学者賞、2014 年 4 月 15 日「地球環境シミュレーションにおけるデータ同化の研究」(The Young Scientists' Prize, The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology)
2. 芳村圭, **三好建正**, 金光正郎: 土木学会水工学委員会　水工学論文賞、2014 年 3 月 4 日「アンサンブルカルマンフィルタを用いた水同位体比データ同化に向けた理想化実験」(Hydraulic Engineering Paper Award, Committee on Hydroscience and Hydraulic Engineering, Japan Society of Civil Engineers)

Computational Chemistry Research Unit

1. Team members

Kimihiko Hirao (Unit Leader)
Jong-Won Song (Research Scientist)
Yukio Kawashima (Research Scientist)
Takao Tsuneda (Senior Visiting Scientist)
Rahul Kar (Visiting Researcher)
Bun Chan (Visiting Researcher)

2. Research Activities

Electronic structure calculations are now indispensible for understanding chemical phenomenon even as for experimental chemists. Density functional theory (DFT) is a major tool to tackle chemical phenomenon. DFT efficiently calculates 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 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. LC-DFT also succeeded in describing induced/response properties. Recently, we found that LC-DFT obtains accurate energies of highest occupied molecular orbital (HOMO) and lowest occupied molecular orbital (HOMO). This indicates that prediction of chemical reactions can be done by LC-DFT calculations. The development of LC-DFT had a large impact in theoretical chemistry and the number of researches based on LC-DFT is growing intensively. However, LC-DFT has difficulty in describing photochemical reactions. Photochemical process includes avoided crossing among electronic states, spin-forbidden transitions, and states with high and low spins. These properties cannot be calculated accurately by LC-DFT. Moreover, the HF exact exchange, which remedies the shortcoming of the exchange functional in conventional DFT, requires large computational effort for real systems, which is the bottleneck for large-scale calculation.

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 using on 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. Efficient method of evaluation for Gaussian Hartree-Fock exchange operator for Gau-PBE functional

We previously developed an efficient screened hybrid functional called Gaussian-Perdew–Burke–Ernzerhof (Gau-PBE) [J. Chem. Phys. 135, 071103 (2011)] for large molecules and extended systems, which is characterized by the usage of a Gaussian function as a modified Coulomb potential for the HF exchange. In the previous researches, we found that the adoption of a Gaussian HF exchange operator considerably decreases the calculation time cost of periodic systems while improving the reproducibility of the band gaps of semiconductors. In our recent research, we presented a distance-based screening scheme tailored for the Gaussian HF exchange integral that utilizes multipole expansion for the Gaussian two-electron integrals. We found the new multipole screening scheme helps to save the time cost for the HF exchange integration by efficiently decreasing the number of integrals of, specifically, the near field region without incurring substantial changes in total energy. In our assessment on the periodic systems of seven semiconductors, the Gau-PBE hybrid functional with a new screening scheme has 1.56 times the time cost of a pure functional while the previous Gau-PBE was 1.84 times and HSE06 was 3.34 times.

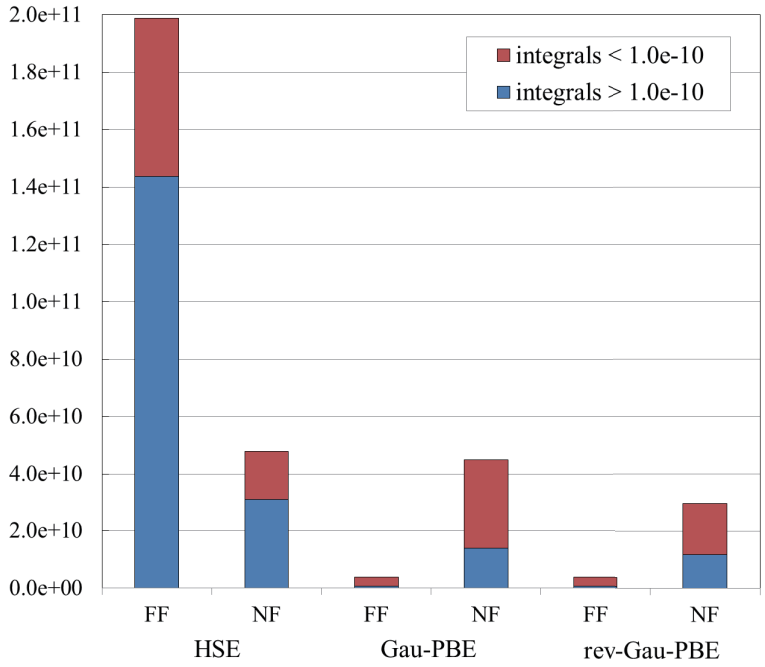


Figure 1 The numbers of calculated HF exchange integrals of HSE, Gau-PBE, and rev-Gau-PBE in C diamond. The numbers of integrals are decomposed into far-field (FF) and near-field (NF) and into integral sizes using the standard of 10^{-10}.

3.2. Long-Range Corrected Density Functional Theory with Linearly-Scaled Hartree-Fock

Exchange Using a Two-Gaussian Operator [LC-ωPBE(2Gau)]

Since the advent of hybrid functional in 1993, it has become a main quantum chemical tool for the calculation of energies and properties of molecular systems. Following the introduction of long-range corrected hybrid scheme for density functional theory a decade later, the applicability of the hybrid functional has been further amplified due to the resulting increased performance on orbital energy, excitation energy, non-linear optical property, barrier height, and so on. Nevertheless, the high cost associated with the evaluation of HF exchange integrals remains a bottleneck for the broader and more active applications of hybrid functionals to large molecular and periodic systems. In this research, we proposed a very simple yet efficient method for the computation of long-range corrected hybrid scheme. It uses a modified two-Gaussian attenuating operator instead of the error function for the long-range HF exchange integral. As a result, the two-Gaussian HF operator, which mimics the shape of the error function operator, reduces computational time dramatically and enables linear-scaling with system size, while maintaining the improved features of the long-range corrected density functional theory.

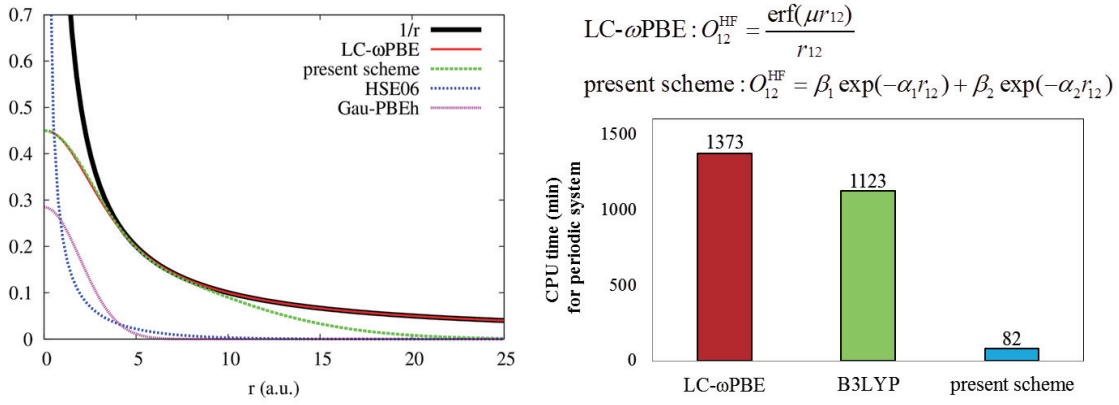


Figure 2 Modified forms of the $1/r_{12}$ operator for the HF exchange contributions and timings (min) for C diamond in the LC-ωPBE, present scheme [LC-ωPBE(2Gau)], Gau-PBEh and HSE06 functionals.

3.3. Assessment of Density Functionals for the Estimation of Enthalpies of Formation, Barrier Heights, and Ionization Potentials of Selected C1-C5 Oxygenates

We assessed B3LYP, BHandHLYP, MPW3LYP, MPW1K, MPWB1K, BB1K, MPW1B95, BMK, LC-ωPBE, LC-BOP, LCgau-BOP, LC-BOP12, LCgau-B97 density functionals and the composite CBS-QB3 method for the enthalpies of formation for some selected oxygenates . Compared to experiment, BMK, LC-ωPBE, LC-BOP, LCgau-BOP, LC-BOP12, LCgau-B97, MPW195, MPW3LYP functionals and CBS-QB3 give root mean square errors (RMSE) in enthalpies of formation no greater than 4 kcal/mol, whilst MPW1K and BHandHLYP show much worse

performance (RMSE of 20 - 40 kcal/mol). The B3LYP, MPWB1K and BB1K results fall between the two extremes. Energy barriers for the dominant paths in the unimolecular decomposition of simple esters (HCO2CH3, C2H5CO2C2H5), C1-C3 acids, and 1-butanol are reproduced well by CBS-QB3, BMK, BB1K, LCgau-B97, and PW1B95 (RMSE= 1- 2 kcal/mol), while other LC methods (LC-ωPBE, LC-BOP, LCgau-BOP, and LC-BOP12) show a deviation of up to 4 kcal/mol. For the ionization potentials, calculated from Koopman's theorem, all of the investigated LC-methods give good results compared to other DFT functionals with a maximum deviation of 0.4 eV, except for LCgau-B97, which has an RMSE of 0.7 eV.

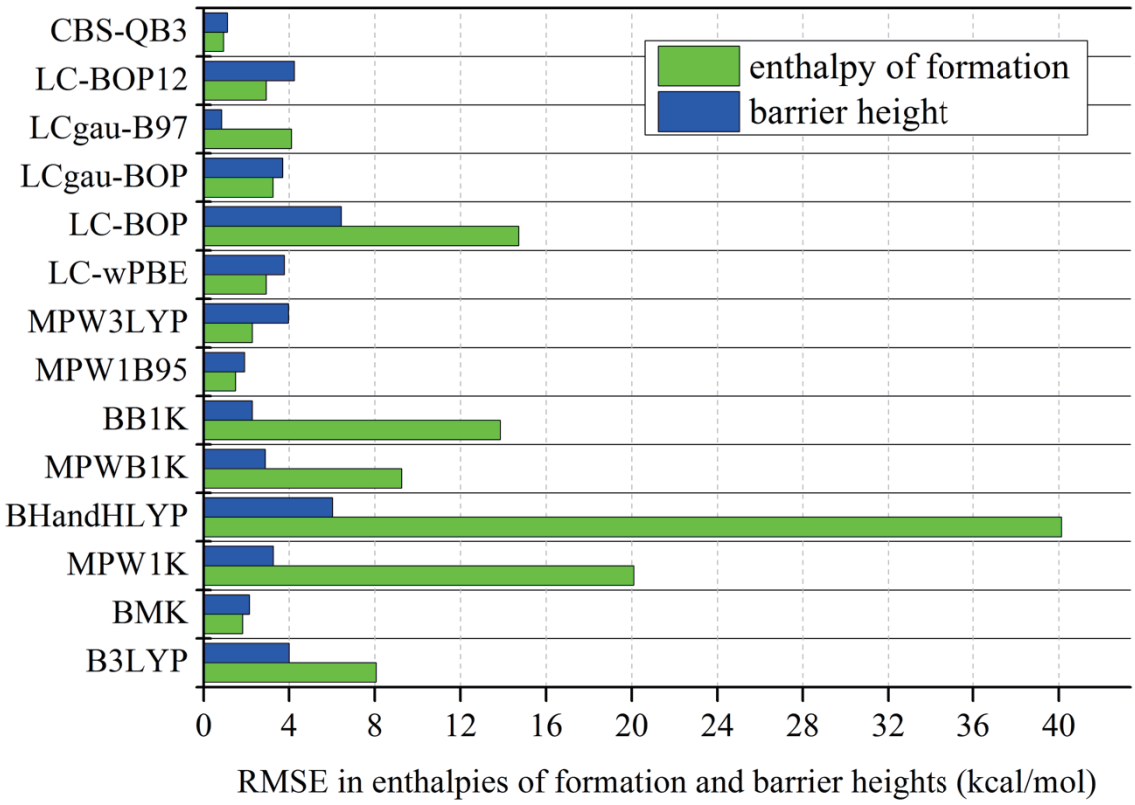


Figure 3 Plot of RMSE in enthalpies of formation and barrier heights for some oxygynates.

3.4. Molecules relevant for Organic Photovoltaics: A Range Separated Density Functional Study

Accurate determination of both fundamental and optical gap is necessary for designing molecules relevant for organic photovoltaics. In this research, we studied how range separated density functionals reproduce frontier orbital energies, HOMO (highest occupied molecular orbital) - LUMO (lowest unoccupied molecular orbital) gaps and optical gaps for molecules relevant for organic photovoltaics. Then, we considered 12 different range separated density functional for computing

HOMO energy, HOMO-LUMO gap and optical gap, which were then compared with available experimental and reported GW values. We found that the reproduction of desired photovoltaic properties primarily depends on range separation parameter. Moreover, the tested functionals are comparable with OT-BNL functional.

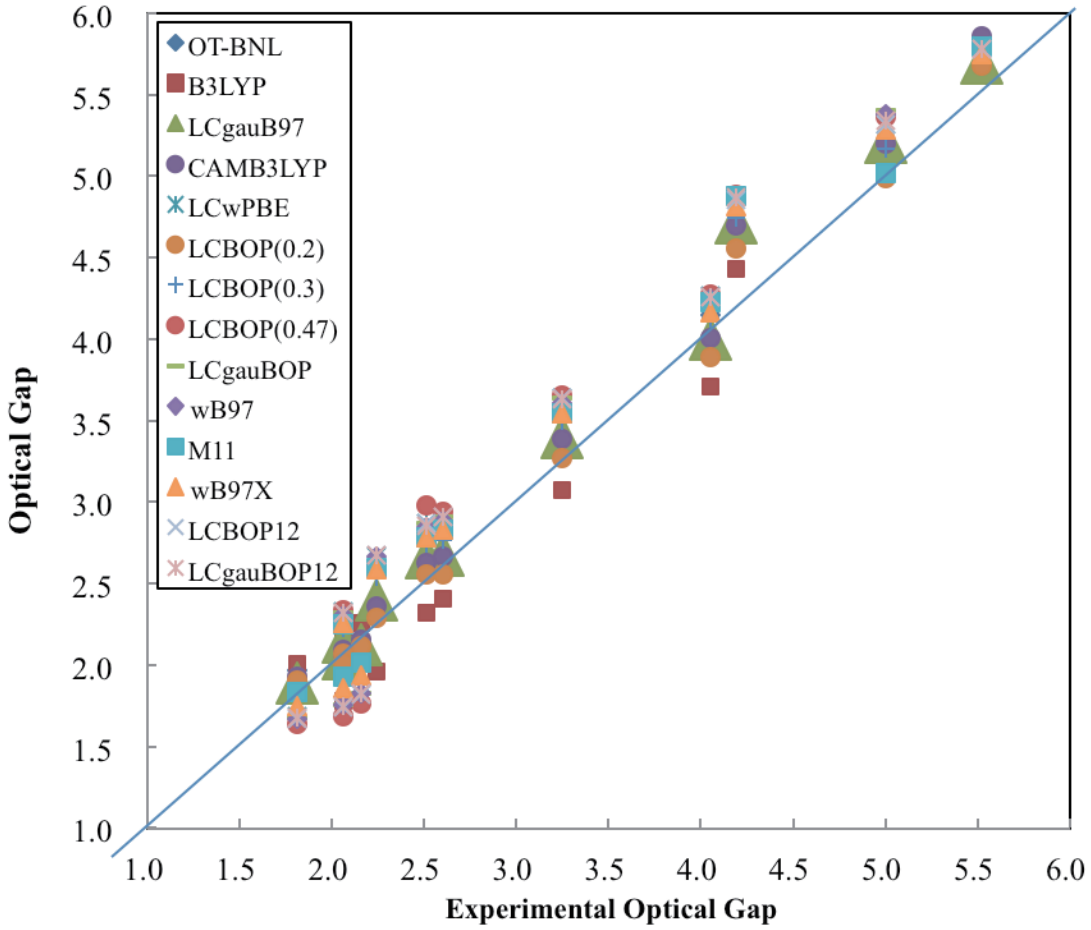


Figure 4 Plot of experimental optical gap versus optical gap (in eV) of large molecules using different rang-separated functionals.

3.5 An approach toward the complete range separation of non-hybrid exchange-correlational

Density functional theory (DFT) is arguably the most popular type of procedures among the various computational chemistry protocols, as these methods provide reasonable accuracy with good computational efficiency. DFT procedures contain an exchange component and a correlation component. Hybrid DFT procedures, which are now the most commonly used DFT, replace a proportion of the DFT exchange with Hartree Fock (HF) exchange. Many hybrid DFT methods are the so-called global hybrids, which have the same proportion of HF exchange throughout the entire

system. However, short-range qualities in a system may have different requirements on the theoretical methods than long-range features. To this end, we previously developed a different type of hybrid DFT, the range-separated DFT (RS-DFT), which uses varying amounts of HF exchange for short-range and long-range interactions. Indeed, such a partition scheme often leads to an improved performance when compared with the typical global hybrids. Most commonly, in conjunction with the RS hybrid DFT exchange, the same correlation functional is used in RS-DFT procedures. Thus, a good performance across the board necessitates a good performance of the correlation functional in all ranges. This begs the question: would it be beneficial to also adopt range separation to the correlation component in an RS-DFT? In the present investigation, we will explore this issue. A different aspect regarding hybrid DFT is that the inclusion of HF exchange leads to an increase in computational cost, when compared with pure DFT procedures that do not have such a component. We thus find it desirable to first focus on pure functionals in the development of such a new DFT protocol. We emphasize that the objective of this study is to introduce a strategy that can complement existing techniques for DFT development, rather than devising the best-performing procedure using this new methodology.

In this study, we use a very simple scheme to achieve range separation of a total exchange–correlation functional. We have utilized this methodology to combine a short-range pure DFT functional with a corresponding long-range pure DFT, leading to a "Range-separated eXchange–Correlation" (RXC) scheme. By examining the performance of a range of standard exchange–correlation functionals for prototypical short- and long-range properties, we have chosen B-LYP as the short-range functional and PBE-B95 as the long-range counterpart. The results of our testing using a more diverse range of data sets, including S12L set of host-guest complexes shown in Figure 5, show that, for properties that we deem to be short-range in nature, the performance of this prescribed RXC-DFT protocol does resemble that of B-LYP in most cases, and vice versa. Thus, this RXC-DFT protocol already provides meaningful numerical results. Furthermore, we envisage that the general RXC scheme can be easily implemented in computational chemistry software packages. This study paves a way for further refinement of such a range-separation technique for the development of better performing DFT procedures.

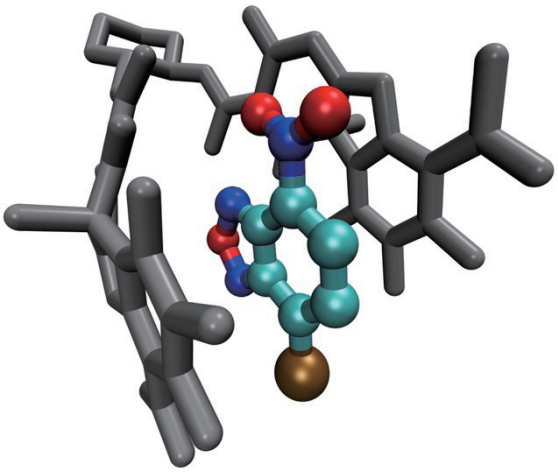


Figure 5. The largest host-guest system used for assessment in S12L set. Hydrogen atoms are omitted.

4. Schedule and Future Plan

In the next fiscal year, we will continue our effort to expand the capabilities of LC-DFT. First, we will develop the order-*N* calculation algorithm of LC-DFT to calculate large molecular systems quantitatively with much less computational time. We have gained insight on how to reduce the time-consuming exact exchange calculation and we will apply our knowledge to the algorithm development. 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, Gau-PBEh, and LC-DFT(2Gau) 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. "Relativistic Density Functional Theory", *J. Comput. Chem. Jpn* **13**, 71-82 (2014).
2. "Towards the Complete Range Separation of Non-Hybrid Exchange–Correlation Functional" Bun Chan, J.-W. Song, Y. Kawashima, and K. Hirao, *J. Comput. Chem.* **36**, 871-877 (2015).
3. "Assessment of hybrid, meta-hybrid-GGA, and long-range corrected density functionals for the anstimation of enthalpies of formation, barrier heights, and ionisation potentials of selected C1–C5 xygenates" A. M. El-Nahas, J. M. Simmie, A. H. Mangood, K. Hirao, J.-W. Song, M. A. Watson, T. Taketsugu, and N. Koga, *Mol. Phys.* (Special Issue in Honour of Nicholas C. Handy) (2015) [**DOI:** 10.1080/ 00268976.2014.1002552].
4. "Is the structure of hydroxide dihydrate $OH^-(H2O)_2$? : An ab initio path integral molecular dynamics study" Y. Ogata, Y. Kawashima, K. Takahashi, M. Tachikawa, *Theo. Chem. Acc.* **134**, 1587 (2015).
5. "Theoretical study on the stability of double-decker type metal phthalocyanines, $M(Pc)_2$ and $M(Pc)_2^+$ (M = Ti, Sn and Sc): critical assessment on the performance of density functionals" M. Sumimoto, Y. Kawashima, K. Hori, H. Fujimoto, *Phys. Chem. Chem. Phys.* **17**, 6478-6483 (2015).
6. "Quantum simulation for muoniated and deuterated methyl radicals in implicit water solvent: combined ab initio path integral molecular dynamics and the polarizable continuum model simulation study" K. Yamada, Y. Kawashima, M. Tachikawa, *Mol. Sim.* [**DOI:** 10.1080/08927022.2014.938070].

7. ”Reactivity index based on orbital energies”, T. Tsuneda, R. K. Singh, *J. Comput. Chem.* **35**, 1093-1100 (2014).
8. “A new electron-nucleus correlation functional for multi-component density functional theory”, T. Udagawa, T. Tsuneda, M. Tachikawa, *Phys. Rev. A* **89**, 052519 (2014).
9. “Theoretical Investigation of Local Proton Conductance in Proton Exchange Membranes for Fuel Cells”, R. K. Singh, T. Tsuneda, K. Miyatake, M. Watanabe, *Chem. Phys. Lett.* **608**, 11-16 (2014).
10. “Chemical reaction analyses based on orbitals and orbital energies” T. Tsuneda, *Int. J. Quant. Chem.* **115**, 270-282 (2015).
11. “Theoretical Study of Isotope Enrichment Caused by Nuclear Volume Effect”, M. Abe, M. Hada, T. Suzuki, Y. Fujii, K. Hirao, *J. Comput. Chem. Jpn* **13**, 92-104 (2014).
12. “Theoretical Study on Reaction Mechanisms of Nitrite Reduction by Copper Nitrite Complexes: Towards Understanding and Controlling Possible Mechanisms of Copper Nitrite Reductase”, S Maekawa, T Matsui, K Hirao, Y Shigeta, *J. Phys. Chem. B* (2015) [**DOI:** 10.1021/acs.jpcb.5b01356].
13. “Long-Range Corrected Density Functional Theory with Linearly-Scaled Hartree-Fock Exchange Using a Two-Gaussian Operator [LC-ωPBE(2Gau)]” J.-W. Song, K. Hirao, *J. Phys. Chem. Lett.* submitted.
14. “Molecules relevant for Organic Photovoltaics: A Range Separated Density Functional Study” R. Kar, M. P. Borpuzari, J.-W. Song, K. Hirao, *Mol. Phys.* submitted.
15. “Efficient evaluation method for Hartree-Fock exchange of Gaussian operator for Gau-PBE functional” J.-W. Song, , K. Hirao, *J. Chem. Phys.* submitted.

(2) Books

1. “Density functional theory for Coordination Chemistry”, T. Tsuneda, Books from Japanese Society of Coordination Chemistry 10 “Quantum and computational chemistry for metal complex systems”, Ed. K. Yamaguchi, S. Sakaki, H. Masuda (2014)

(3) Invited Talks

1. “Present and Future Status of Quantum Chemistry”, T. Tsuneda, 3rd Frontier Chemistry Center (FCC) International Symposium, Hokkaido Univerisity, July 13-14 (2014).
2. “Looking Toward Quantum Chemistry on the Exascale”, T. Tsuneda, US-Japan Workshop on Exascale Applications, Gatlinburg, Tennessee, Sep. 5-6 (2014).
3. “Orbital energy gaps vs excitation energies for extended systems”, T. Tsuneda, 10th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2014), Casa Piedra Santiago, Oct. 5-10 (2014).

4. “Relationship between excitation energies and orbital energy gaps for large systems”, T. Tsuneda, The 9th International Conference on Computational Physics (ICCP9), The National University of Singapore, Jan. 7-11 (2015).
5. “On the difference between band gaps and orbital energy gaps”, T. Tsuneda, A cluster of topical meeting on Current Trends in Condensed Matter Physics (CTCMP) 2015, National Institute of Science Education and Research (NISER), Bhubaneswar, Feb. 19-22 (2015).
6. “The present and the future of theoretical chemistry”, T. Tsuneda, 42nd Hokkaido University Theoretical Chemistry Seminar, Hokkaido University, Jun. 12 (2014). (In Japanese)
7. “The K Computer and Computational Chemistry”, K. Hirao, 102nd Indian Science Congress -Advances in Computation of Electronic Structure ACES-2015, University of Mumbai, Jan. 4 (2015).
8. “Quantum chemical approach to elucidate the mechanism of metabolism and UV protection”, Y. Kawashima, CBI Annual Meeting 2014 (Focused Session: Metabolomics and First-Principle Calculation: Prediction and Validation), Tower Hall Funabori, Tokyo, Oct. 29 (2014). (In Japanese)
9. “Towards large scale computing of path integral molecular dynamics simulation”, Y. Kawashima, The 12th Inamori Frontier Workshop: Large scale computing technology towards practical application, Kyushu Universtiy, Jan. 23 (2015). (In Japanese)
10. “Development of DFT functional applicable to large molecular and periodic systems” J.-W. Song, CJK-WTCC-II conference, Kobe, Jan. 20-23 (2015).

(4) Posters and presentations

1. “Tackling Nuclear Quantum Effect in Quantum Chemistry”, Y. Kawashima, XIXth International Workshop on Quantum Systems in Chemistry and Physics, Tamsui, Nov. 13 (2014).
2. ”Analysis of HF exact exchange in Long-Range Corrected Density functional Theory”, Y. Kawashima, K. Hirao, 17th Annual Meeting of Theoretical Chemistry, Nagoya University, May 22-24 (2014). (Poster in Japanese)
3. ”Theoretical Study of $OH^-(H_2O)_2$ Cluster Considering Nuclear and Thermal Fluctuation Effects”, Y. Ogata,Y. Kawashima, K. Takahashi, M. Tachikawa, 15th Annual Meeting of Theoretical Chemistry, Nagoya University, May 22-24 (2014). (In Japanese)
4. ”Analysis of HF exact exchange in Long-Range Corrected Density functional Theory Calculation of Physical Properties”, Y. Kawashima, K. Hirao, The 8th Annual Meeting of Japanese Society for Molecular Science, Hiroshima University, Sep. 21-24 (2014). (Poster in Japanese)

5. “Efficient evaluation of short-range Gaussian attenuation Hartree-Fock exchange for periodic systems and large molecules” J.-W. Song, K. Hirao, ICCMSE, Athens, Mar. 20-23 (2015).
6. “Efficient evaluation of short-range Gaussian attenuation Hartree-Fock exchange for periodic systems and large molecules” J.-W. Song, M. A. Watson, K. Hirao, Molecular Electronic Structure, Amasya, Sep. 1-5 (2014).
7. “Analysis of the difference in intra- and inter-molecular charge transfer employing long-range corrected density functional theory”, J.-W. Song, K. Hirao, The 17th Theoretical Chemistry Symposium, Nagoya University, May22-24. (In Japanese)

(5) Patents and Deliverables

- None

Computational Disaster Mitigation and Reduction Research Unit

1. Team members

Muneo Hori (Unit Leader)
Hideyuki O-tani (Postdoctoral Researcher)
Jian Chen (Postdoctoral Researcher)
Kohei Fujita (Visiting 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:
1) A next generation urban area model will use a few Geographical Information Systems (GIS). A serious bottle neck of using different GIS's is that each system has its own coordinate system. For data stored in different GIS's, therefore, we have to connect data using a common coordinate system. A methodology of establishing connection based on "Land Address" is developed. The methodology extracts a polygon which is separated by Ward Boundary, and then associates the polygon to the common coordinated system, using string data and the local coordinate. Based on this methodology, we develop a prototype of a module which automatically connects data in different GIS's.
2) Liquefaction is a ground failure which is induced by sudden rise of underwater ground pressure when strong ground motion hits loosened sand. Since the governing equations are found for this coupling problem, we study the stability of the solution and show that it is anisotropy and particle detaching that loses the stability when a *seed* of liquefaction starts to grow; we make linear perturbation analysis for the governing equation, simplifying non-linear properties of soil deformation. Using a finite element program, we numerically confirm that while anisotropy produces temporal increase in water pressure, particle detaching spreads water pressure increase spatially.
3) It is inevitable to use high performance computing in solving earthquake disaster problems for a larger urban area subjected to ground motion with long duration. In particular, ground motion amplification processes which take place in surface ground layers with complicated configuration needs analysis of a high fidelity model of the layers which needs large scale computation. Together with HPCI Strategic Program for Innovation Research Field 3, we have developed a non-linear finite

element program for ground motion amplification analysis. It is shown that the developed program is capable to analyze a model of a few ten billion degree-of-freedoms, which is the largest in this class of problems, using the full system of K computer.

3. Research Results and Achievements

3.1. Development of next-generation urban model for Kobe city

In constructing a next generation urban area model, we will have to use a few Geographical Information Systems (GIS). There is a serious bottle neck of using different GIS's, since each system has its own coordinate system; each object in a target area has different *local* coordinate of a GIS, according to which the object is located in it. Therefore, it is necessary to connect data for one object which are stored in different GIS's.

We are developing a methodology of establishing connection based on Land Address (an address managed by the national government to specify the land use). The methodology takes the following procedures: 1) it extracts a polygon for Land Address which is separated by Ward Boundary (a line which separates zone of one Land Address); 2) it seeks local coordinate and string data which are related to the polygon; and 3) it assigns the polygon to a common coordinate, using the local coordinate and the string data. It should be noted that unlike easiness of manual processing of seeking a common coordinate, automated and robust processing is difficult since there are many cases for the spatial relation between the polygon and the local coordinate.

Based on this methodology, we have developed a prototype of a module which automatically connects data of one object stored in different GIS's. The current target is an object for a residential house or building; see Fig. 3.1.1. We extract data for such a structure which are stored in a commercial GIS and a GIS managed by a local government, in order to construct an analysis model for seismic response analysis. Robustness is essential for this data extraction. In visualizing the seismic response, we have to convert the results of the seismic response analysis in the form that commercial software of visualization is able to process. Flexibility is essential for this data conversion since there a few choices of the commercial software. The prototype is developed to eliminate or minimize manual processing of the data extraction and conversion.

As the number of GIS's increases and more objects are processed, the efficiency of data extraction and conversion needs to be improved. In Fig. 3.1.2, we show a schematic view of the improving the efficiency in which the architecture of the program is changed. It is natural to use data processing such as extraction and conversion as subsidiary functionality in applying the numerical computation. However, the architecture based on this standard treatment cannot make high efficiency, as it needs frequent communication with the numerical analysis method. Hence, we change the architecture so that direct read/write for the data processing is realized. This treatment makes the data processing a major functionality rather than a subsidiary functionality. While coding is tough to exclude manual

Fig. 3.1.1 Extracted data for Land Address. Red lines stand for Ward Boundary and polygons surrounded by red lines are an area of Land Address.

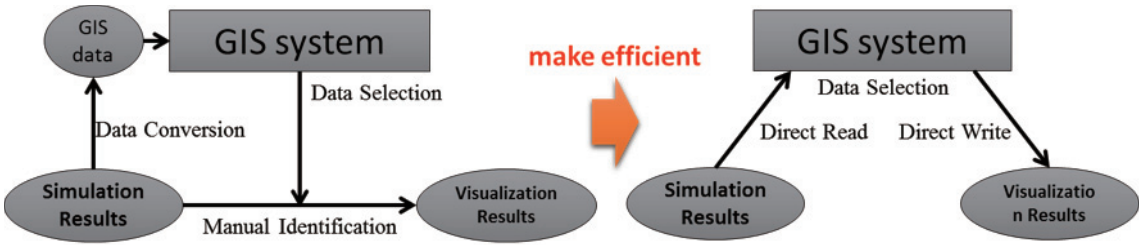


Fig. 3.1.2 Improvement of the efficiency in the GIS data processing with interactive selections.

processing, the present prototype succeeds to make efficient data processing.

3.2 Numerical simulations for stability analysis of liquefaction

In the fiscal year of 2013, we showed that dilatancy played a key role in the stability of the solution of the governing equation of a dynamic problem of soil-water coupling. We obtained a theoretical threshold value for the dilatancy at which liquefaction was initiated.

3.2.1 Mathematical model

We start from the governing equations of a dynamic problem of soil-water coupling. Denoting by $\boldsymbol{u}$ and p the perturbations of the increment of soil displacement and water pressure, we write the governing equation as

$$\begin{aligned} \rho \mathrm{D}^2 \boldsymbol{u} - \boldsymbol{\nabla} \cdot (\boldsymbol{c} : \boldsymbol{\nabla} \boldsymbol{u}) + \boldsymbol{\nabla} p = \boldsymbol{0}, \\ \boldsymbol{\nabla} \cdot \mathrm{D} \boldsymbol{u} - \boldsymbol{\nabla} \cdot (k \boldsymbol{\nabla} p) = 0, \end{aligned} \tag{3.2.1}$$

where ρ, $\boldsymbol{c}$, and k are density, elasto-plasticity and permeability; $\boldsymbol{\nabla}$ and D stand for spatial and temporal differentiation; and $\cdot$ and : denote the first- and second-order contraction.

As for dilatancy of soil, we introduce anisotropy of elasticity. Here, isotropy means that $c_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$, with (λ, μ) and δ_{ij} being Lame's constants and Kronecker's delta, and anisotropy means non-zero components which relate shear deformation to normal stress, say, $c_{1112} = c_{1113} = c_{1211} = c_{1311} = \alpha$.

Applying the Fourier transform of Eq. (3.2.1) with the kernel of $\exp(i(\boldsymbol{\xi} \cdot \mathbf{x} - \omega t))$, we derive the follow characteristic equation for frequency ω and wave number $\boldsymbol{\xi} = \xi(1,0,0)$:

$$r^4 + i r_k r^3 - (1 + r_s^2) r^2 - i r_k r_s^2 r + r_s^2 - 2 r_a^4 = 0, \tag{3.2.2}$$

where r is the non-dimensional frequency, i.e., $r = \omega / \omega_p$ and $r_{s,a,k} = \omega_{s,a,k} / \omega_p$ with

$$\omega_p = \xi \sqrt{\tfrac{\lambda + 2\mu}{\rho}}, \quad \omega_s = \xi \sqrt{\tfrac{\mu}{\rho}}, \quad \omega_\mathrm{a} = \xi \sqrt{\tfrac{\alpha}{\rho}} \text{ and } \omega_k = \tfrac{1}{\rho k}.$$

If the imaginary part of r is positive, it means an unstable solution since it grows exponentially with respect to time. The critical value of the dilatancy ratio is given as

$$r_a = \sqrt[4]{\frac{\mu}{2(\lambda + 2\mu)}}, \tag{3.2.3}$$

which can be seen in Fig. 3.2.1(b) as an example.

3.2.2 Numerical simulation for spherical perturbations

In the fiscal year of 2014, we have developed and verified a two-dimensional finite element code, which is able to analyze the stability of the governing equation. We use this code for the stability analysis for perturbations in the full three-dimensional settings. The problem setting chosen is for the spherical growth of a perturbation.

Here we only show the unstable solution for a relative large dilatancy ratio. Material prosperities used for simulation are summarized in Table 3.2.1. The results for stable solutions please refer to the related publication. The governing equations are solved numerically in a finite cubic domain (with edge length $L = 0.01$ m) for a spherically symmetrical initial perturbation. The time for a wave with velocity $c_p = 231.46$ m/s propagates from the center to the boundary of the domain is taken as the reference time, denoted by T. As shown in Fig. 3.2.2, the unstable solution is developed when the initial perturbation starts to propagate from the center to the boundary of the domain.

A consequence of the unstable solutions is the concentration of stress, as shown in Fig. 3.2.3. The first stress invariant, $I_1 (= \sigma_{kk})$, and the second invariant of the deviatoric stress, $J_2 (= \sigma_{ij}\sigma_{ij}/2 - (\sigma_{kk})^2/6)$, are plotted. As is seen, due to the unstable solution, the stress invariants around the center region are accumulated. Further investigations are needed to clarify the possibility of the

propagation of the unstable solution considering the formation of "micro cracks", weakening of soil strength when the accumulated stresses exceed a certain yield criterion.

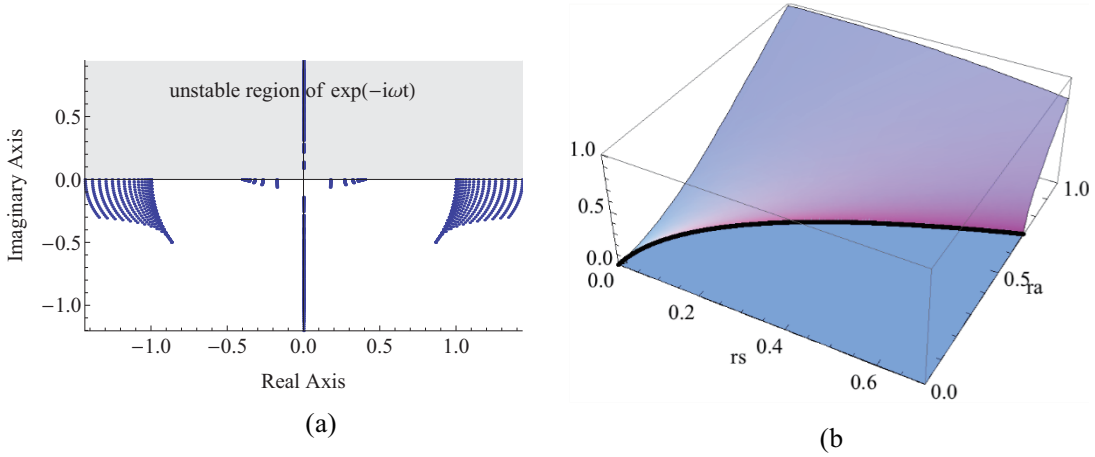
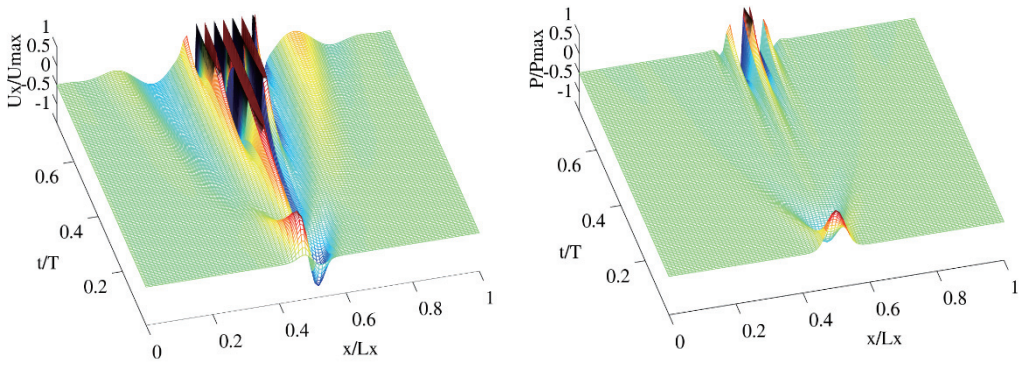


Fig. 3.2.1 Results of theoretical analysis: (a) r on the complex plane for a fixed $r_s = 0.4$ and varying r_k and r_a between 0 and 1. (b) Imaginary part of r and critical dilatancy ratio r_a (indicated as the thick black line) for $r_k = 0.1$, with negative values of the imaginary part truncated as zero.

Table 3.2.1. Material properties for code verification

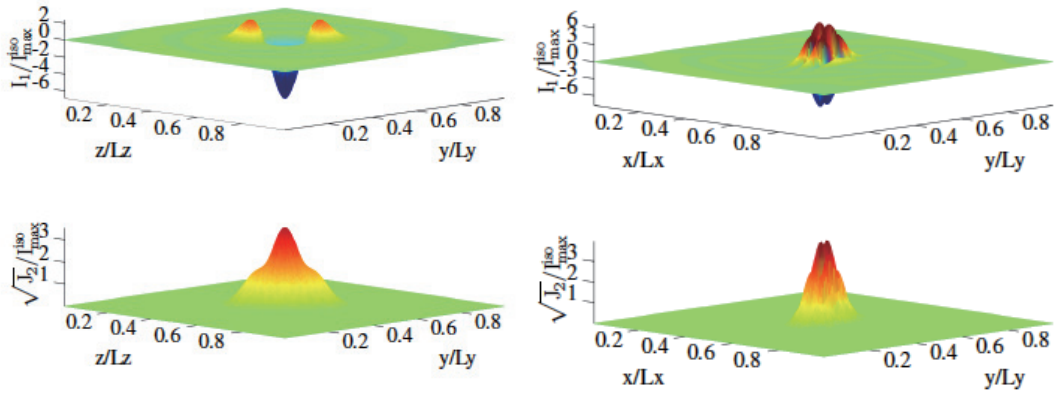
Young's modulus E (MPa)	Poisson's ratio v	Density ρ (kg/m^3)	Permeability k (m^{3}s/kg)	Dilatancy ratio r_a
50	0.4	2000	1.02e-8	$\sqrt{0.30}$

3.3 Numerical simulations for ground motion and seismic response of urban area



(a) (b)

Fig. 3.2.2 Displacement and pressure distribution at the center line ($y = z = L/2$) of the domain: (a) displacement u_x and (b) pressure p. U_{max} and P_{max} are computed from the same simulation settings without considering dilatancy.



(a) (b)

Fig. 3.2.3 Stress invariant at the center planes at $t/T = 0.74$: (a) $x = L/2$ and (b) $y = L/2$. The reference value I_{max} is computed from the same simulation settings without considering dilatancy.

Earthquake hazard and disaster which take place in an urban area are physical processes the mechanisms of which are fully clarified. Due to wide area and long time of the entire processes, it requires large scale numerical computation. Moreover, a model of high fidelity is needed in order to fully capture detailed geometrical configuration of the area and heterogeneous material properties. A three-dimensional finite element method is a unique choice of the numerical analysis, even though

simpler analysis methods such as finite difference method have been used with approximation of topographical effects on the physical processes.

High performance computing that is realized by K computer is a computer resource that is able to carry out the large scale numerical computation of the three-dimensional finite element analysis, even though the analysis uses unstructured grid in order to model non-smooth configuration of the target. In this fiscal year, together with HPCI Strategic Program for Innovation Research Field 3, we have developed a fast solver which is fast and scalable for a sparse matrix.

3.3.1 Formulation of finite element method

The wave equation of solid continuum is the common governing equation for the physical processes of the earthquake hazard and disaster. This equation is converted to the following discretized equation for the finite element method:

$$\left(\frac{4}{\mathrm{d}t^2}\boldsymbol{M}+\frac{2}{\mathrm{d}t}\boldsymbol{C}^n+\boldsymbol{K}^n\right)\delta\boldsymbol{u}^n=\boldsymbol{F}^n-\boldsymbol{Q}^{n-1}+\boldsymbol{C}^n\boldsymbol{v}^{n-1}+\boldsymbol{M}\left(\boldsymbol{a}^{n-1}+\frac{4}{\mathrm{d}t}\boldsymbol{v}^{n-1}\right). \quad (3.3.1)$$

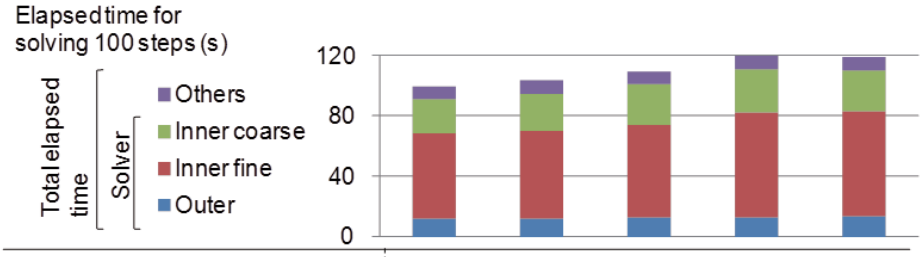
where $\boldsymbol{M}$, $\boldsymbol{C}$ and $\boldsymbol{K}$ are mass, damping and stiffness matrices, respectively, $\delta\boldsymbol{u}$, $\boldsymbol{u}$, $\boldsymbol{v}$, $\boldsymbol{a}$, $\boldsymbol{F}$ and $\boldsymbol{Q}$ are incremental displacement, displacement, velocity, acceleration, external force and unbalanced force vectors, respectively, $\mathrm{d}t$ is time increment, and superscript n stands for the value at the time step (a matrix with superscript n changes due to the material non-linearity). The material non-linearity of soil uses the Ramberg-Osgood model and the Masing rule.

Most of computation time in the finite element method is to compute $\delta\boldsymbol{u}^n$ by solving Eq. (3.1.1). Therefore, it is essential to develop a solver for this equation. A modern supercomputer consists of numerous computation nodes which do not share memory, and it is important to reduce numerical manipulation as well as to minimize inter-node communication in order to achieve large scale and fast numerical computation. Conjugate gradient method (CG) is suitable for parallel computation since it does not require all node computation and all node communication. Hence, there are many improved solvers which are based on CG method.

In applying such a solver, suitable pre-conditioning is needed to improve the nature of the target matrix equation. As is seen in Eq. (3.3.1), the matrix for $\delta\boldsymbol{u}^n$ has a term of $(4/\mathrm{d}t^2)\boldsymbol{M}$, which becomes dominant in the matrix for smaller $\mathrm{d}t$. The convergence of CG method thus is faster, compared with the static problem which ignores the inertia effect. The matrix components change at each time step, and pre-conditioning of decomposing the matrix for $\delta\boldsymbol{u}^n$ becomes computationally expensive. Pre-conditioning which does not require large computation is standard in solving Eq. (3.3.1). We adopt multi-grid and mixed precision for reducing computation and communication for fast finite element solver.

3.3.2 Numerical experiment of earthquake hazard and disaster simulation

The performance of the developed finite element method is shown in Fig. 3.3.1. The scalability of the solver (or the developed finite element method) is good up to the full K computer system. Using this scalable solver we make a numerical simulation of part of Tokyo Metropolis; the size of the area is 3.5 x 3.5 km. The target frequency is 15 Hz, which implies the smallest element size of 0.66 m for the wave velocity of 100 m/s. A model of high fidelity is constructed with the total 40.1 x 10^9 degree-of-freedoms. 1995 Hyogo Earthquake (JMA Kobe) is used as input ground motion, the duration of which is 15 s, and the time increment and the total time step are $dt = 0.001$ s and 15,000, respectively. The full system of K computer is used for this simulation. The natural hazard and disaster simulation is visualized as ground motion distribution and structural seismic response distribution in Fig. 3.3.2. Such visualization will play a role of next-generation hazard map for earthquake.



# of CPU cores (# of compute nodes)	36,864 (4,608)	73,728 (9,216)	147,456 (18,432)	294,912 (36,864)	663,552 (82,944)
Degrees-of-freedom (billion)	1.5	3.0	6.0	12.0	27.0
Degrees-of-freedom per CPU core	41k	41k	41k	41k	41k
Performance of solver (% to peak)	14.49	14.06	13.28	11.82	12.34

Fig. 3.3.1 Size-up scalability of developed finite element method (GAMERA). Elapsed time is for solving 100 time steps of non-linear computation

4. Schedule and Future Plan

In the fiscal year of 2015, we plan to make a next-generation hazard map for Kobe City, using the module of GIS data processing which will be developed by improving the prototype conversion and the numerical analysis methods which are developed together with HPCI Strategic Program for Innovation Research Field 3. We plan to include the following two ingredients: 1) lifeline for water and sewage, which consists of buried pipelines; and 3) ground failure which are induced by liquefaction. For these ingredients, numerical analysis methods developed by expert researchers will be plugged in the integrated system. The key issues are summarized as follows:

1) Construction of next generation urban area model which include lifeline network and underground.
2) Execution of earthquake hazard and disaster simulation based on numerous earthquake scenario
3) Smart visualization of numerical simulation results; if each simulation will produce 10 GB data, we have to deal with 10 TB data for 1,000 earthquake scenarios.

5. Publication, Presentation and Deliverables

(1) Journal Papers

1. Hideyuki O-TANI, Jian CHEN and Muneo HORI: a Template-Based Floor Shape Recognition Applied to 3D Building Shapes of GIS Data, Journal of Japan Society of Civil Engineers, Ser. A1, Vol.70, No.4, I_1124-I_1131, 2014.
2. Hideyuki O-TANI, Jian CHEN and Muneo HORI: Automatic Combination of the 3D Shapes and the Attributes of Buildings in Different GIS Data, Journal of Japan Society of Civil Engineers, Ser. A1, Vol.70, No.2, I_631-I_639, 2014.

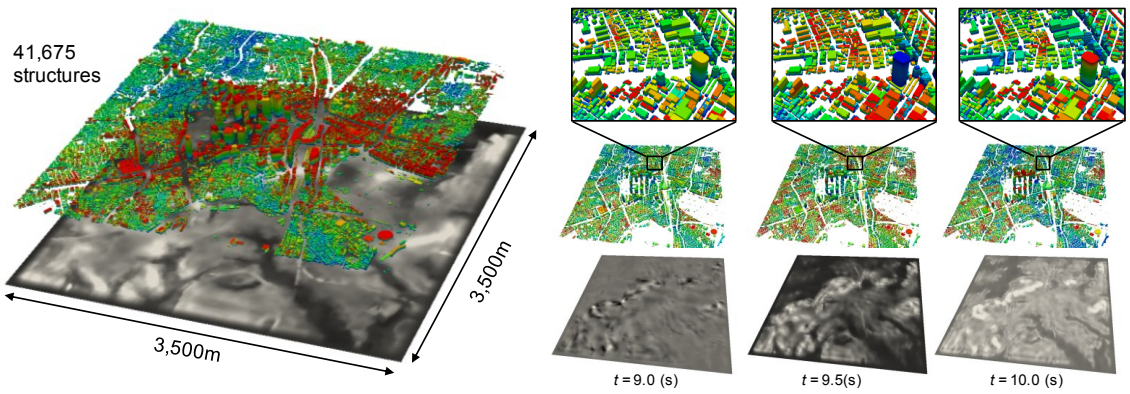


Fig. 3.3.2 Earthquake hazard and disaster simulation for an urban area. Three snapshots are for the distribution of the ground motion and the structural seismic responses at designated time step.

3. Jian Chen, Hideyuki O-tani and Muneo Hori, On mathematical stability analysis of liquefaction considering soil-water coupling, Journal of Japan Society of Civil Engineers, Ser. A2 (Applied Mechanics (AM)), vol.70, No.2, I_641-I_648, 2014.
4. Hans-Georg Matuttis and Jian Chen, Understanding the Discrete Element Method: Simulation of Non-Spherical Particles for Granular and Multi-body Systems, Wiley, 2014.
5. Tsuyoshi Ichimura, Kohei Fujita, Seizo Tanaka, Muneo Hori, Maddegedara Lalith, Yoshihisa Shizawa and Hiroshi Kobayashi: Physics-based urban earthquake simulation enhanced by 10.7 BlnDOF x 30 K time-step unstructured FE non-linear seismic wave simulation, Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC '14), Pages 15-26, Gordon Bell Finalist, 2014. 10.1109/SC.2014.7.
6. Tsuyoshi Ichimura, Kohei Fujita, Muneo Hori: Nonlinear Seismic Ground Response Analysis of Local Site Effects with Three-Dimensional High-Fidelity Model, Encyclopedia of Earthquake Engineering, pages 1-8, 2014. 10.1007/978-3-642-36197-5_60-1.
7. Kohei Fujita, Tsuyoshi Ichimura, Muneo Hori, Lalith Wijerathne and Seizo Tanaka: A quick earthquake disaster estimation system with fast urban earthquake simulation and interactive visualization, Procedia Computer Science (The International Conference on Computational Science 2014), Vol. 29, pp. 866-876, 2014. doi:10.1016/j.procs.2014.05.078.
8. Shunsuke Homma, Kohei Fujita, Tsuyoshi Ichimura, Muneo Hori, Seckin Citak and Takane Hori: A physics-based Monte Carlo earthquake disaster simulation accounting for uncertainty in building structure parameters, Procedia Computer Science (The International Conference on Computational Science 2014) , Vol. 29, pp. 855-865, 2014. doi:10.1016/j.procs.2014.05.077.

(2) Conference Papers

1. Jian Chen, Hideyuki O-tani and Muneo Hori, Stability Analysis for Local Liquefaction Initiation of Plane Wave Type, Computer Methods and Recent Advances in Geomechanics, Oka, Murakami, Uzuoka & Kimoto (Eds.), p. 661-666, Taylor & Francis Group, 2015 (14th IACMAG)
2. Kohei Fujita, Tsuyoshi Ichimura, Muneo Hori, Lalith Maddegedara and Seizo Tanaka: Scalable multicase urban earthquake simulation method for stochastic earthquake disaster estimation, Procedia Computer Science (The International Conference on Computational Science 2015), Accepted, 2015.
3. Kohei Fujita, Tsuyoshi Ichimura, Seizo Tanaka, Muneo Hori, Maddegedara Lalith: Numerical Convergence Analysis of Three-dimensional Nonlinear Earthquake Wave Amplification Simulation, Proceedings of The First International Conference of IASUR:

Sustainable Society as Our Challenge, Pages 327-334, 24-27 October 2014.

4. Abdurrahman Sahin, Kohei Fujita, Muneo Hori, Mehmet Ozan Yilmaz: Application of Integrated Earthquake Simulation for the Zeytinburnu District of Istanbul, Computational Engineering and Science for Safety and Environmental Problems (COMPSAFE 2014), 13-16 April 2014.
5. Kohei Fujita, Tsuyoshi Ichimura, Muneo Hori, Lalith Wijerathne, Seizo Tanaka: Urban Earthquake Simulation with Large-Scale 3D Ground Motion Analysis and Structural Response Analysis, Computational Engineering and Science for Safety and Environmental Problems (COMPSAFE 2014, keynote), 13-16 April 2014.
6. Shunsuke Homma, Kohei Fujita, Tsuyoshi Ichimura, Muneo Hori, Seckin Citak, Takane Hori: Many Case Simulation for Estimating Urban Earthquake Disaster Accounting Uncertainties in Structure Models, Computational Engineering and Science for Safety and Environmental Problems (COMPSAFE 2014), 13-16 April 2014.

(3) Invited Talks

1. Jian Chen, Hideyuki O-tani, Kohei Fujita and Muneo Hori, An Application of High Performance Computing: Stability Analysis for Soil Liquefaction, Tongji University, Shanghai, Dec. 25, 2014.

(4) Posters and presentations

1. Hideyuki O-TANI, Jian CHEN and Muneo HORI: Template-Based Automatic Construction of Building Models from GIS data, COMPSAFE 2014, Sendai, 16, April 2014.
2. Hideyuki O-TANI, Jian CHEN and Muneo HORI: Association between 3D Shapes and Attributes Contained in Two Different Types of GIS Data, JSCE symposium on applied mechanics, Okinawa, Japan, 11, May 2014.
3. Hideyuki O-TANI, Jian CHEN and Muneo HORI: Automatic Construction of Urban Model for Disaster Simulation from Urban 3D Map and Official Building Registry, The 14th Japan Earthquake Engineering Symposium, Chiba, Japan, 4, December 2014.
4. Jian Chen, Hideyuki O-tani and Muneo Hori, Stability Analysis for Local Liquefaction Initiation of Plane Wave Type, 14th IACMAG International Conference, Kyoto, Sep.22-25, 2014 (Oral presentation).
5. Jian Chen, Hideyuki O-tani and Muneo Hori, Stability Analysis of Liquefaction Considering Soil-Water Coupling, The 5th AICS International Symposium, Kobe, Dec 08-09, 2014 (Poster presentation).
6. Jian Chen, Hideyuki O-tani and Muneo Hori, Stability Analysis of Liquefaction Considering Soil-Water Coupling, 2015 Symposium on the Application of Mechanics to Geophysics,

San Diego, Jan.17-18, 2015 (Poster presentation).

7. Jian Chen, Hideyuki O-tani and Muneo Hori, Stability Analysis of Wave Propagation for Investigation of Triggering Conditions of Liquefaction, COMPSAFE2014, Sendai, Apr.13-16, 2014 (Oral presentation).
8. Jian Chen, Hideyuki O-tani and Muneo Hori, On Mathematical Stability Analysis of Liquefaction Considering Soil-Water Coupling, 17th Applied Mechanics Symposium, JSCE, Naha, May 10-11, 2014 (Poster presentation).

(5) Patents and Deliverables

Computational Structural Biology Research Unit

1. Team 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.

A variety of experimental techniques exist toward this goal. X-ray crystallography has been the primary tool to study protein conformations, providing high-resolution structures. Even though cryo electron microscopy (EM) provided lower resolution data, it has provided critical information on structure and dynamics of large biological molecules. More recently, efforts like 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, at the current experimental condition, it cannot achieve atomic level resolution such as obtained by X-ray crystallography.

Computational approaches are valuable under this situation, since they could provide information that is not accessible from experiments. 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. In particular, we are developing hybrid analysis that combines low-resolution experimental data as obtained from, such as, cryo-EM and XFEL, with computational methods that utilizes high performance computers, such as K computer. These tools help us to acquire knowledge on the structure of physiologically important protein complexes that are unattainable with existing experimental techniques, and in the longer term 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. In previous years, we had developed a new method, Hybrid Electron Microscopy Normal Mode Analysis (HEMNMA) that utilizes molecular mechanics algorithms to simulate conformational dynamics and use the resulting conformations to extract the dynamical information from cryo-EM images. In order to make this method more accessible to the general public and to facilitate its usage, a friendly graphical interface was developed with the Xmipp framework. Three modules (normal mode analysis, flexible alignment and advanced results analysis) are available (see Figure 1) and all HEMNMA analysis can be performed using this new graphical interface.

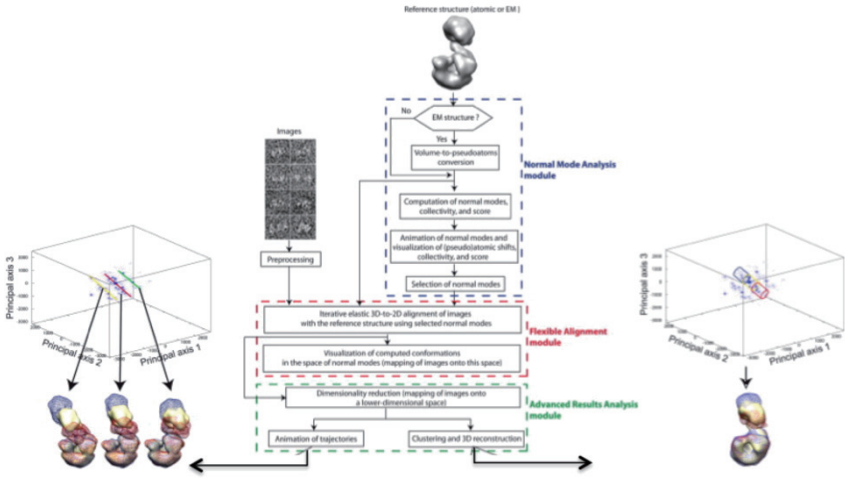


Figure 1: Modules available in the HEMNMA graphical interface and example of analysis that can be performed. (Adapted from CO. Sorzano et al. J. Struct. Biol. (2014))

In addition, we discussed the application of this method to the dynamics of the Tomato Bushy Stunt Virus (TBSV), which is a small icosahedral plant virus known to undergo conformational rearrangements upon change in pH conditions. 4000 particles images and three symmetric normal modes, which reflect the icosahedral arrangement of the virus, were considered for HEMNMA approach. The analysis showed that images could be classified into 5 classes representing different conformation of the virus, with the primary conformational change consisting in a radial expansion of the virus particle consistent with previous experiments. Such conformations were used to discuss in more details the conformational change.

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. Numerous computational tools have been developed to interpret conformational change observed in cryo-EM data (flexible fitting).

Using multiple flexible fitting methods can be a useful approach to evaluate the accuracy of models by comparing difference in their resulting model conformation. While flexible fitting methods can produce accurate atomic models, there are not always successful. In some particular cases, several of these methods consistently fail. In light of such results, to obtain a better understanding of the behaviors observed in these fittings and evaluate the limitation of the flexible methods, a more comprehensive survey of the fitting performance is performed using multiple initial fitting conditions.

Our flexible fitting approach was implemented in GENESIS (Dr. Sugita's team). Running multiple simulations (320 different conditions) revealed that accurate models are not consistently obtained (Figure 2, No REUS). Therefore we implemented a new scheme to perform flexible fitting, which relies on replica exchange simulation, a method that enables better conformational sampling. In such approach, *n* simulations are run concurrently with *n* different force constant. Conformations are allowed to exchange between these simulations, therefore experiencing different force constant and enhancing sampling (REUS). Without REUS (No REUS in Figure 2) most models have low accuracy (RMSD ~6Å) while with REUS, all models have an RMSD around 2.5Å RMSD. Therefore, appropriate conformational sampling is critical to obtain accurate model and using REUS can improve accuracy of the models.

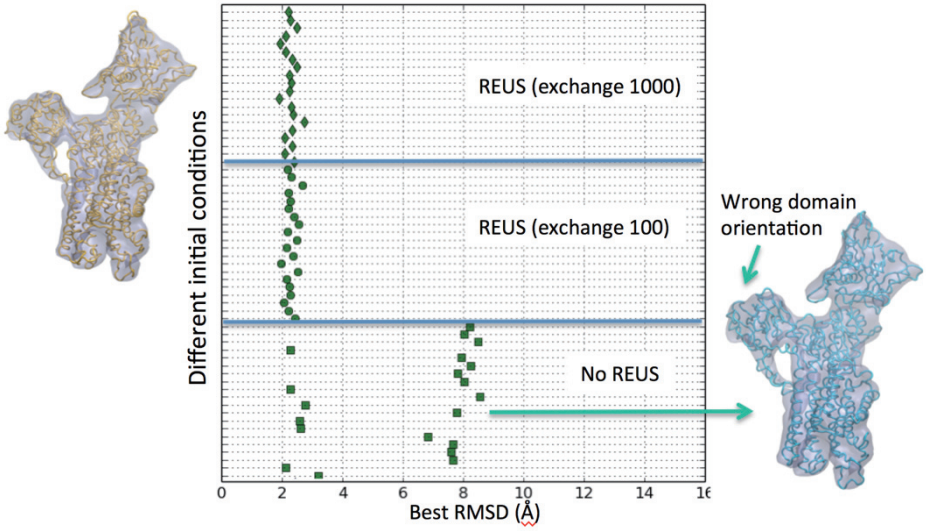


Figure 2: Best RMSD with the target structure obtained from multiple simulations. Without REUS, atomic models might not be accurate (high RMSD observed). Using REUS, atomic models within 2. 5Å are consistently obtained.

3.3. Collaboration on X-ray diffraction imaging

In this fiscal year, we have started a collaboration with Dr. Song (RIKEN SPring-8 Center, Imaging Development Team) on RNA sponges, which are assembled from small interfering RNA molecules. RNA sponges are biologically relevant as they can silence gene expression. Dr. Song and collaborators collected data on RNA sponges using coherent diffraction imaging. Our group was in charged of reconstructing the overall shape of the molecules using computational tools. The first overall 3D structure of a RNA sponge was described (Figure 3). Even though the structure is low resolution, it revealed a core with higher density suggesting a higher organization or a core more packed than the surface.

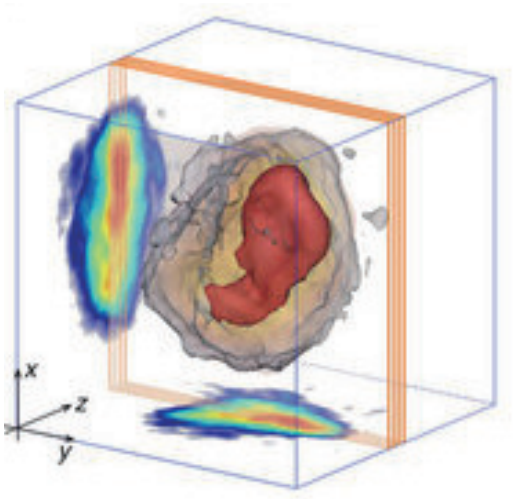


Figure 3: Complete 3D structure of a microsponge is shown. The overall shape is displayed transparently (grey) in order to visualize the internal dense region (red). Projection densities along xz-plane and yz-plane are superposed. Adapted from M. Gallagher-Jones et al. (2014) Nat Commun. May 2;53798

3.4. Computational tools to analyze XFEL experimental data

We are also developing tools to analyze XFEL data in order to obtain structural information of biological molecules. In particular, we aim to develop computational algorithms that would provide the shape of the biological systems. 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. Such algorithm is better suited to current XFEL single particle experiments targeted on μm scale systems, such as organelles and small cells.

Previously, we performed "fitting" studies i.e. an atomic model is created by deforming other known structures. However, for these μm scale systems, such an approach would not be suitable. Therefore, we have started to work on ab initio structure modeling from XFEL diffraction patterns, which can propose a structure model, though at low-resolution, from the data alone. We chose gold particles as a model system for the first test case. Such model system is often used for initial testing in experiments and many data are available, therefore it is a good candidate to develop a new approach. Preliminary data on a small system composed of three gold colloids shows that actual arrangements can be obtained by comparing the target X-ray diffraction pattern with the patterns from candidate model structures (Figure 4).

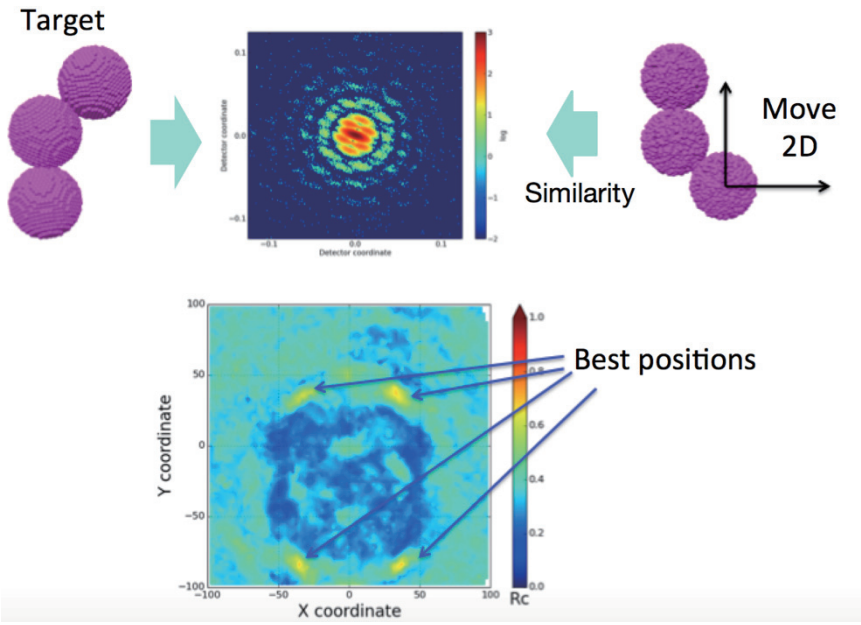


Figure 4: Comparison between target diffraction pattern and candidate models as one gold colloid is moved in X and Y directions.

3.5. Collaboration

We are collaborating with Dr. Sugimoto's group (FIBER, Konan University) and Dr. Tanaka (Kobe University) to study the effects of solvent properties on DNA thermal stability. Detailed atomic molecular dynamics simulations on DNA molecules adopting different conformations with different

co-solute concentrations were performed. Such studies revealed new insights (effect of co-solute, water-DNA and co-solute-DNA interactions) for a better understanding of the thermal stability of DNA structures in a molecular crowding environment, which is critical to understand physiology in vivo.

4. Schedule and Future Plan

We are planning to continue to develop tools to analyze XFEL data in order to obtain structural information of 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.

One emphasis of our research is the description of the dynamics of biological molecules through the development of computational tools to characterize low-resolution experimental data. We intend to continue and establish new collaborations with experimental groups in Japan and abroad in order to study structure, function and dynamics of biological molecules.

Finally, on the longer term we plan to establish a computational framework to build structures from low-resolution structural data without a priori knowledge of the overall structure of the molecular complexes. Such approach would integrate multiple types of experiments, multiple types of computational methods (multi-scale modeling and simulations, protein structure prediction, protein-protein interactions…). Such framework would be important to study structure/function and dynamics of biological molecules.

5. Publication, Presentation and Deliverables

(1) Journal Papers

1. M. Gallagher-Jones, Y. Bessho, S. Kim, J. Park, S. Kim, D. Nam, C. Kim, Y. Kim, Y. Noh do, O. Miyashita, F. Tama, Y. Joti, T. Kameshima, T. Hatsui, K. Tono, Y. Kohmura, M. Yabashi, SS. Hasnain, T. Ishikawa, C. Song. (2014) Macromolecular structures probed by combining single-shot free-electron laser diffraction with synchrotron coherent X-ray imaging. **Nat Commun**. 2:5:3798
2. S. Patel, E. Vierling and F. Tama. (2014) Replica exchange molecular dynamics simulations provide insight into substrate recognition by small heat shock proteins. **Biophys J**. 10:2644-55
3. Hybrid Electron Microscopy Normal Mode Analysis graphical interface and protocol. (2014) CO. Sorzano, J.M. de la Rosa-Trevín, F. Tama, S. Jonić. **J. Struct. Biol**. 188:134-41

(2) Conference Papers

1. Q. Jin, C.O. Sanchez Sorzano, I. Callebaut, F. Tama, S. Jonic (2014). Elastic image registration to fully explore macromolecular dynamics by electron microscopy. In: Image Processing (ICIP), IEEE International Conference on, 27-30 Oct. 2014, 2075-2079

(3) Invited Talks

1. Computational tools to characterize structure of biological molecules from low-resolution data. Novel measurement techniques for visualizing 'live' protein molecules at work - Kickoff Symposium. October 2014. Kyushu University, Japan.
2. Structure modeling with EM and XFEL data. Osamu Miyashita, Atsushi Tokuhisa, Florence Tama. Coarse-Grained Modeling of Structure and Dynamics of Biomacromolecules 3. August 2014. Telluride workshop. USA

(4) Posters and presentations

1. Examination of *ab* initio structural modeling for the pattern matching method using X-ray free electron laser. Atsushi Tokuhisa, Osamu Miyashita, Florence Tama. Annual Meeting of the Biophysical Society of Japan. September 2014. Sapporo, Japan.
2. Hybrid Approach for X-Ray Free Electron Laser Single Particle Analysis of Biomolecular Systems Osamu Miyashita, Atsushi Tokuhisa, Florence Tama. Keystone Symposia. Hybrid Methods in Structural Biology. March 2015. Tahoe City, USA

(5) Patents and Deliverables

Facility Operations and Development Team

1. Team members

Toshiyuki Tsukamoto (Team Head)
Masami Kurokawa (Technical Staff)
Mitsuru Tanaka (Technical Staff)
Hiroyuki Takitsuka (Technical Staff)
Katsuyuki Tanaka (Technical Staff)
Satoru Matsushita (Technical Staff)

2. Research Activities

The K computer facilities have many features not found at other supercomputer sites. These include an expansive and pillar-free computer-room, power supply system that consists of a co-generation system (CGS) and a high-speed current-limiting circuit breaker without uninterruptible power supply (UPS), distribution boards installed not on computer-room walls but under a raised floor, extremely quiet and high-efficiency air conditioners, and water-cooling system for CPUs featuring precise temperature control.

To ensure stable working of K computer and its peripherals, the facility operations and development team (FODT) of the operations and computer technologies division, RIKEN AICS is responsible for operation and enhancement of the facilities. Furthermore, FODT conducts research on the advanced management and operations of AICS' facilities.

One of the most serious problems is rapid and substantial increase in electricity prices since 2011. Therefore, we investigate the most suitable driving conditions for AICS facilities to achieve effective cost reduction.

Another problem is increased power consumption by AICS. The use of electricity by AICS is strictly limited by a contract between AICS and the local electric supply company. However, recently, the facility's power consumption exceeded the contract limit. This matter is important because the company requires us to accept a raise in the upper/lower power limit, which amounts to an increase in electricity cost. To prevent this problem, we have investigated a method to control K computer's power consumption by using emergency job stopping together with the system operations and development team and the software development team of operations and computer technologies division, RIKEN AICS.

3. Research Results and Achievements

3.1. Optimum operation of electric power

Figure 1 shows the trend in the power consumption of AICS and K computer in FY2014, and the status of power supply, which consists of commercial power purchased from a supply company and the power generated by the CGS.

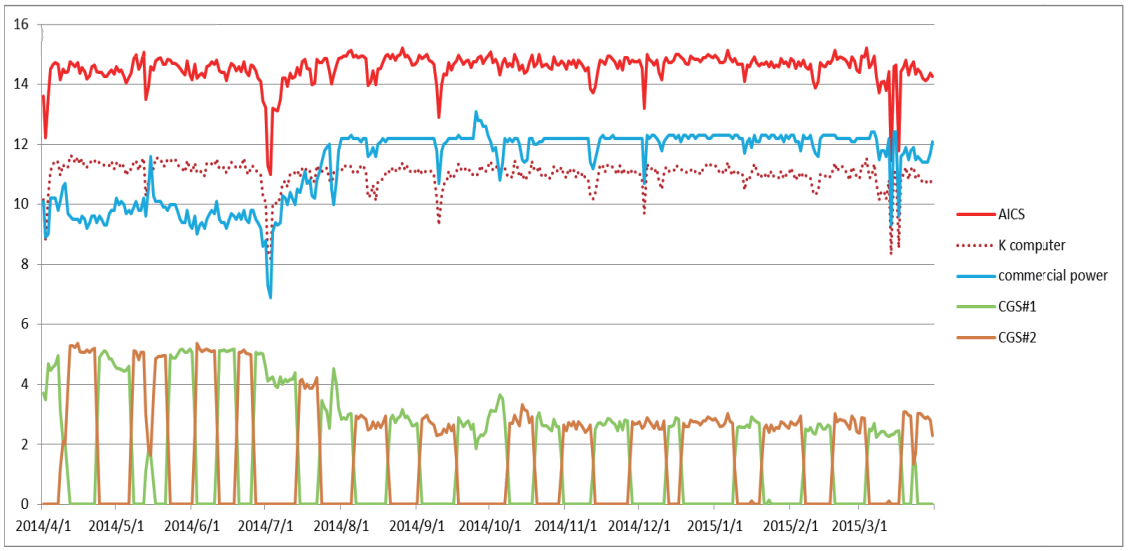


Figure 1 Trend of electric power consumption and supply (FY2014)

The power consumption of AICS is almost synchronized with that of K computer. The power consumption of AICS is nearly 15,000 kW on average, and the power consumption of K computer accounts for approximately 80% (12,000 kW) of AICS' total consumption.

As shown in Figure 1, AICS' electric power supply consists of commercial and CGS power. There are two CGS systems in AICS, and they are used by turn for two weeks at a time. Therefore, at least one CGS is always in use. Commercial electric power is covenanted at 12,750 kW, and power consumption was approximately 12,000 kW (annual average), which corresponds to approximately 90% load factor.

To minimize the cost, we try to optimize the ratio of commercial and CGS electricity.

To investigate the optimized conditions that minimize the sum of electricity and gas cost, we determined the costs of several ratios of commercial electricity to CGS electricity. We also constructed a model to describe energy flow of the electric power supply and cooling system. Then, we performed computer simulation using the model and actual operating data. In FY2015, we intend to clarify the cost-optimized conditions that contribute toward reducing costs.

3.2. Improvements to power usage effectiveness (PUE)

We have continued to work on improvements for the effective use of electricity. PUE is a well known indicator of the effectiveness of electricity use.

To improve PUE, we have attempted to optimize the operation of the air-conditioning system since FY2013.

Figure 2 indicates a change in the annual average power consumption of K computer (including the peripheral devices) and cooling equipment. After FY2013, the power consumption of K computer has been almost flat at approximately 11800 kW, but the power consumption of the equipment decreased gradually from FY2013 to FY2014. Accordingly, the PUE of AICS improved to 1.240 in FY2014 from 1.297 in FY2012, thus contributing to reduction in electricity cost.

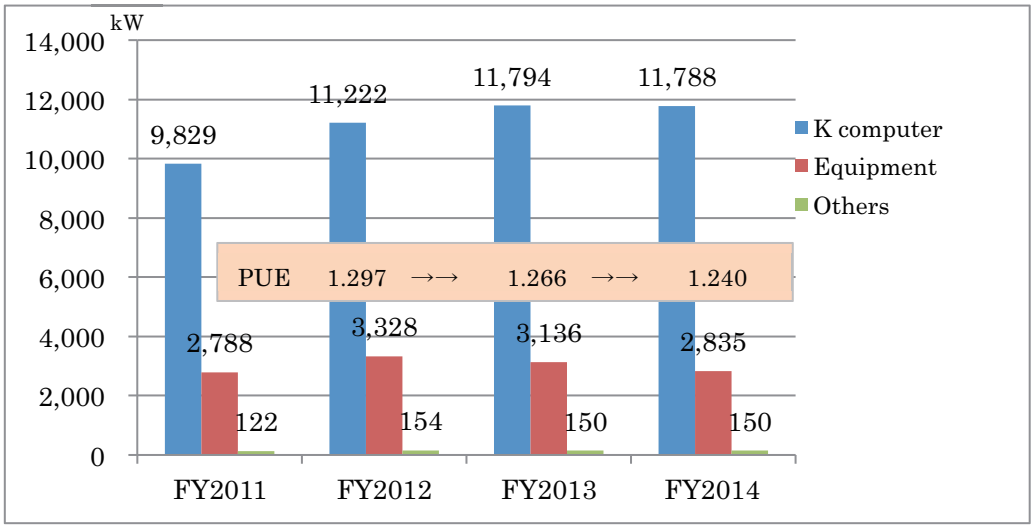


Figure 2 Trend in annual average electric power consumption

In FY2013, we reduced the electricity cost of air-conditioners by reducing the number of working air-conditioners. Total cooling performance was maintained by lowering the air temperature. We could achieve a reduction of 192 kW in power consumption.

In FY2014, we focused on the fault-tolerance feature of the air-conditioning equipment. Each air-conditioner has two motors for fault-tolerance. We found that if one of the two motors could be stopped, airflow could be maintained at approximately 60%. Thus, we reduced power consumption by a further 301 kW.

4. Schedule and Future Plan

We will continue to improve the advanced management and operation of AICS facilities and contribute to the user service of K computer. We will work on reducing costs by investigating and applying the most suitable driving condition to all of the electric power supply and cooling equipment. Furthermore, we will improve electric power control of the entire AICS facility to prevent overshooting the contracted power demand with the system operations and development team.

5. Publication, Presentation, and Deliverables

(1) Journal Papers

1. Keiji Yamamoto, Atsuya Uno, Katsufumi Sugeta, Toshiyuki Tsukamoto, Fumiyoshi Shoji, “スーパーコンピュータ「京」の運用状況,” IPSJ Magazine Vo.55 No.8 pp.786-793, 2014. (In Japanese)

(2) Conference Papers

1. Atsuya Uno, Hajime Hida, Fumio Inoue, Naoki Ikeda,Toshiyuki Tsukamoto, Fumichika Sueyasu, Satoshi Matsushita, Fumiyoshi Shoji, “Operation of the K computer Focusing on System Power Consumption,” HPCS2015, 2015, Japan. (In Japanese) (to appear)
2. Lili Jin, Kouji Yutani, Hiroyuki Yamano, Hiroyuki Takitsuka, Satoshi Matsusita, Toshiyuki Tsukamoto, “計算科学研究機構における設備最適運転条件の検討その２,” Proceedings of the 49th Japanese Joint Conference on Air^conditioning and Refrigeneration(Tokyo). (In Japanese)
3. Satoshi Matsushita, Hiroyuki Takitsuka, Toshiyuki Tsukamoto, “スーパーコンピュータ施設における低騒音空調機の省エネ運用,” Proceedings of the 49th Japanese Joint Conference on Air-conditioning and Refrigeneration(Tokyo). (In Japanese)

(3) Invited Talks

- None

(4) Posters and presentations

1. Fumio Inoue, Atsuya Uno, Toshiyuki Tsukamoto, Satoshi Matsushita, Fumichika Sueyasu, Naoki Ikeda, Hajime Hida, Fumiyoshi Shoji, “電力消費量の上限を考慮した「京」の運用,” IPSJ-SIGHPC 2014-HPC-146 No.4, 2014. (In Japanese)
2. Atsuya Uno, Hajime Hida, Naoki Ikeda, Fumio Inoue, Toshiyuki Tsukamoto, Fumichika Sueyasu, Fumiyoshi Shoji, “「京」におけるジョブ単位の消費電力推定の検討,” IPSJ-SIGHPC 2014-HPC-147 No.20, 2014. (In Japanese)

(5) Patents and Deliverables

- None

System Operations and Development Team

1. Team members

Atsuya Uno (Team Head)
Hitoshi Murai (Research & Development Scientist)
Motoyoshi Kurokawa (Research & Development Scientist)
Keiji Yamamoto (Postdoctoral Researcher)
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 consisting of 82,944 compute nodes. It has played a central role in the High Performance Computing Infrastructure (HPCI) initiative granted by the Ministry of Education, Culture, Sports, Science and Technology. The HPCI has achieved the integrated operation of the K computer and other supercomputer centers in Japan and has enabled seamless access from user machines to a cluster of supercomputers that includes the K computer. Moreover, the HPCI has provided large-scale storage systems that are accessible from all over Japan.

The System Operations and Development Team (SODT) has conducted research and development on advanced management and operations of the K computer. While analyzing operational statistics collected during shared use, the SODT has improved the system configuration, including aspects involving job scheduling, the filesystem, and user environments. For example, achieving higher system utilization is very difficult because the K computer has to process various sizes and types of jobs simultaneously. The SODT has responded flexibly to user requests and analyzed the operational status, thereby realizing a high level of utilization of approximately 75% in FY2014. Moreover, the SODT has developed tools that improve the usability of the K computer.

The K computer's power consumption exceeded the limit several times during FY2013. This is a problem because it forces us to renew the contract-power upper limit, which means expense for the electricity increases. To prevent this increase, the SODT investigated an emergency job-stopping method based on the estimated power consumption of each job using thermal sensors in computer racks.

The SODT also helped users manage the K computer and utilize K computer resources effectively by improving the system software. This support was conducted together with the software development team.

3. Research Results and Achievements

3.1. System software improvements of the K computer

We fixed and improved many aspects of the system software through shared use. Here, we describe the major activities in FY2014.

- Analysis of operation statistics

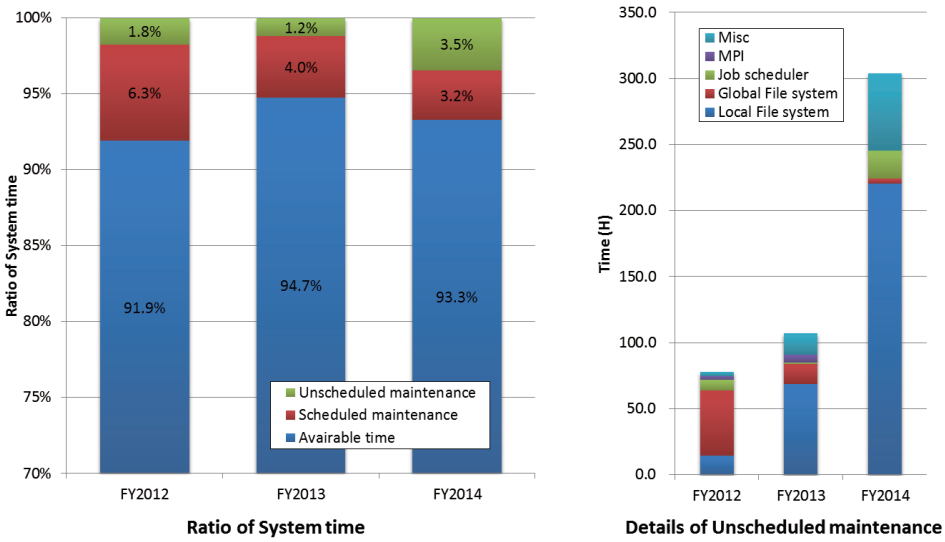


Figure 1 Ratio of system time (left) and details of unscheduled maintenance (right)

Figure 1 shows the ratio of system time (left) and details of unscheduled maintenance (right). Scheduled maintenance primarily consisted of system software updates and maintenance at the end of FY2014, whereas unscheduled maintenance consisted of system unavailability because of unexpected system failures, such as hardware errors, system software bugs, and so on. Overall, we have made the K computer available to users for more than 90% of the time. As the K computer has stabilized, the scheduled maintenance time decreased, but the unscheduled maintenance time in FY2014 was tripled as compared with FY2013. Primarily, the unscheduled maintenance in FY2014 was because of local filesystem failures as the recovery from one local filesystem failure consumes a long time to reconfigure the filesystem. The reduction of such failures is the most important problem that we need to resolve promptly.

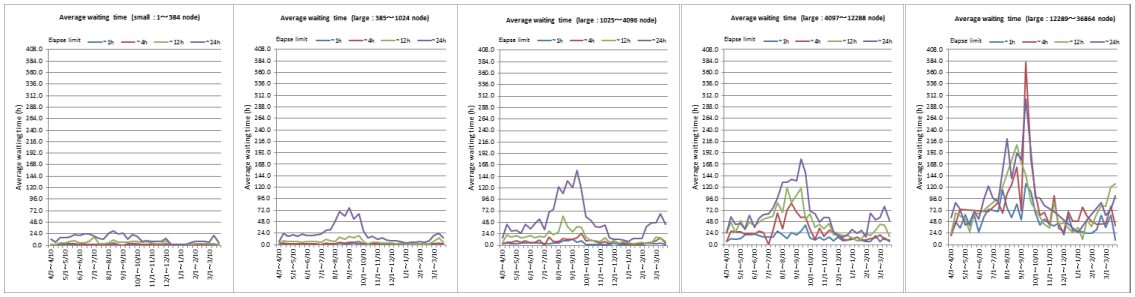


Figure 2 Average waiting times in FY2014

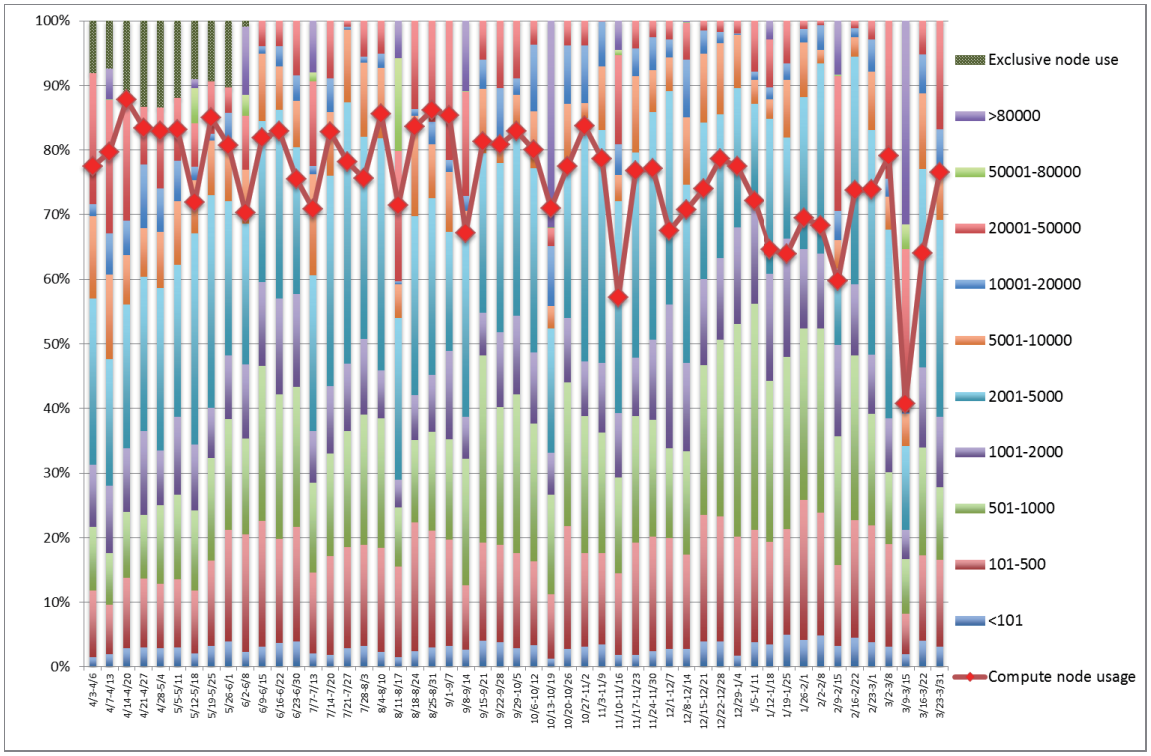


Figure 3 Details of resource usage in FY2014

Figure 2 shows average waiting times with respect to both job sizes and elapsed times in FY2014. The average waiting times were directly proportional to both elapsed time and the number of nodes, indicating that the fairness in job execution has been kept. The average waiting times in September 2014 were substantially longer than those in other months. Each group had appropriate computing resources for a year, and these resources were divided into two terms as follows: (1) from April to September and (2) from October to March. To consume the remaining computing resources before they expire, users tend to submit many jobs at the end of each term. In FY2013, job congestions clearly occurred in August and September 2013 and March 2014, and in FY2014, they occurred during the same months; however, this year's average waiting times were approximately 50%–70% as compared to FY2013. In FY2014, computing resources assigned to users were a few percentage points less than those in FY2013. This decrease led to a significant reduction of the average waiting times in FY2014.

Figure 3 shows resource usage details for FY2014. We achieved approximately 75% node usage in FY2014; more specifically, node usage during the first term of FY2014 was 79%, whereas that during the second term was 72%. If a user uses all the first term's resources within the term, he/she can use the second term's resources also in the first term. Therefore, if too much of the second term's resources are used in the first term, there will be a shortage in the second term's resources. In FY2014, this happened, and the second term's node usage was decreased. To prevent this, for FY2015, we will assign computational resources more than those of FY2014 and less than those of

FY2013; moreover, we will make new rule to suppress the overuse of the second term's resources in the first term.

- Analysis of job scheduling

We analyzed job scheduling on the K computer using a simulator. In FY2014, we evaluated system utilization on the basis of differences in start times of file staging preceding job execution; the results are shown in Figure 4. System utilization increased in the preceding time from 0 to 6 hours, descending from 12 to 24 hours. When the preceding time was long, the compute node assigned to the job were determined earlier; thus, if the compute nodes in which the job could be assigned in an earlier start time were free, the job could not be rescheduled. This means that the preceding time of file staging was one of the important parameters in job scheduling.

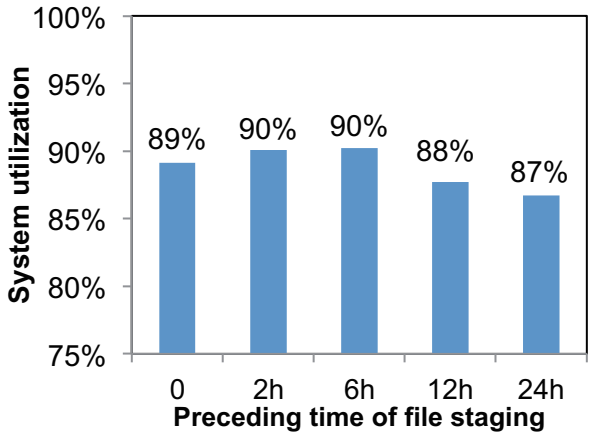


Figure 4 System utilization by time preceding file staging

3.2. Approach for the power consumption problem

The K computer's power consumption exceeded the given limit several times during FY2013; this is an important problem because it forces us to increase the contract-power upper limit, thereby increasing the cost, which cannot be ignored. To prevent this problem, we performed a preliminary review that estimated the power consumption of each job, thereby enabling us to control the overall K computer's power consumption. Moreover, we investigated an emergency job-stopping method based on the estimated power consumption of each job in case power consumption again exceeds the given limit.

- Preliminary review of large-scale jobs

  To prevent power consumption from exceeding the given limit, we performed a preliminary review of large-scale jobs. In this process, we estimated the power consumption of jobs using all compute nodes versus the power consumption of a small-scale job with the same characteristics, thereby permitting users to submit jobs if the estimated power consumption is below the limit.

- Emergency job-stopping method

When power consumption exceeds the given limit, we have to stop the jobs to reduce it. To select the appropriate jobs to be stopped, we proposed a method to estimate the power consumption of each job using thermal sensors in computing racks. By this method, we estimated the job's power consumption using CPU and exhaust air temperature variations. Figure 5 shows the relation between the assigned number of nodes and estimated power consumption of each job during a two-day period from June 11 to June 12, 2014. The upper figure shows the number of compute nodes assigned to each job, indicated by the blue line. The lower figure shows the estimated power consumption of each job, with the red line indicating the observed K computer's power consumption. In both the upper and lower figures, areas with the same color during the same period correspond to the same job. The width of an area denotes the elapsed time from start to termination of the job. The white areas under the blue or red lines indicate all jobs using less than 1,000 compute nodes. From these figures, we note that the estimated power consumption of each job is not proportional to the size of assigned compute nodes, and our proposed method is useful in selecting the appropriate jobs to be stopped.

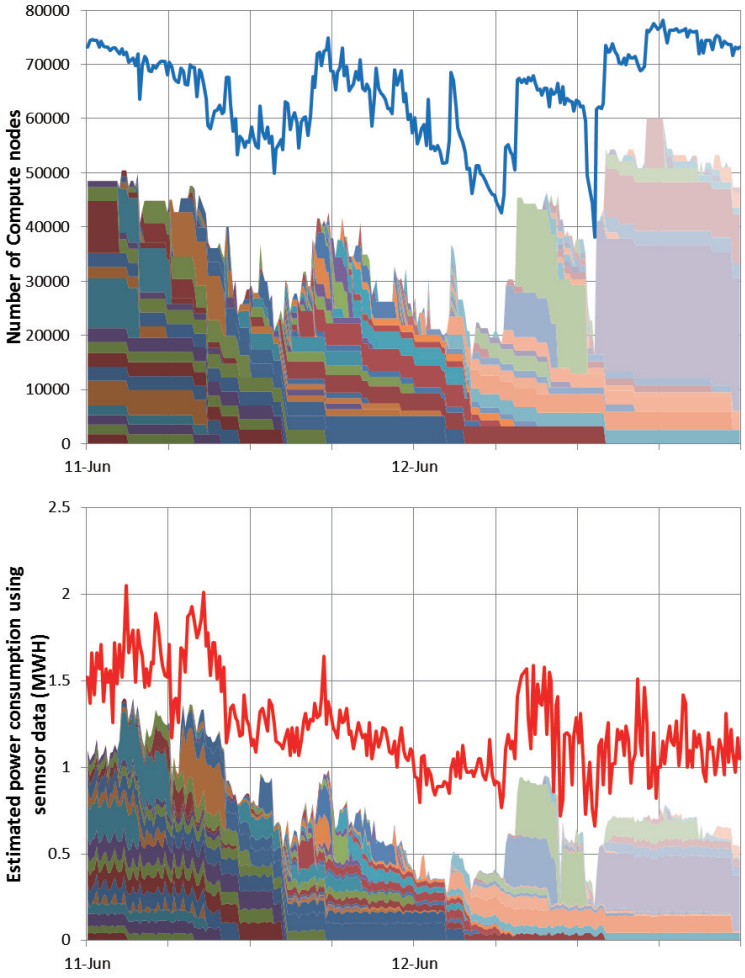


Figure 5 Assigned number of nodes (upper) and estimated power consumption (lower)

3.3. User support

We conducted user support such as consulting services.

- Number of users

  The K computer has over 130 groups and over 1,500 users as of the end of March 2015. The total number of HPCI users and AICS researchers is approximately 1,250 and 250, respectively. The number of daily active users is approximately 110.

- Consulting services

  We supported users through the K support desk, providing users technical information on the K computer, including system environment, system tools, software libraries ,etc. Our consulting services were offered together with the software development team. Figure 6 indicates the number of issues in FY2014, showing the number of new issues in FY2014 to be approximately 170. The number of new issues in FY2013 is approximately 230. Because users have learned how to use the K computer and various approaches and workarounds for problems, we consider the number of new issues to be decreased.

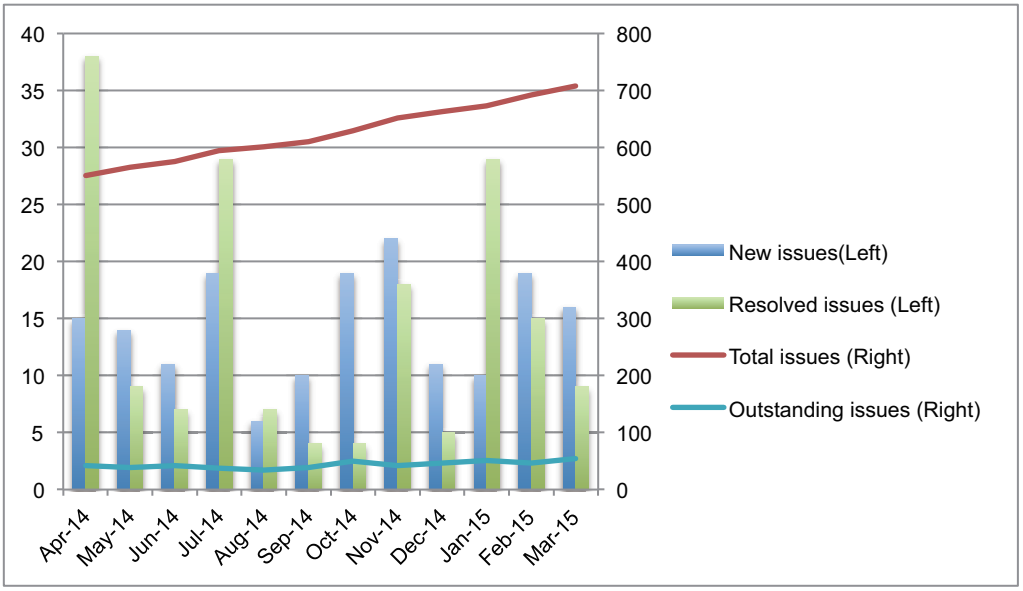


Figure 6 Number of issues in FY2014

4. Schedule and Future Plan

We continue to improve the system software of the K computer and provide user support. Improved system software that improves the usability of the K computer will be released in FY2015. Moreover, we have investigated an approach for the K computer's power consumption problem in terms of job scheduling.

5. Publication, Presentation, and Deliverables

(1) Journal Papers

2. Keiji Yamamoto, Atsuya Uno, Katsufumi Sugeta, Toshiyuki Tsukamoto, Fumiyoshi Shoji, “スーパーコンピュータ「京」の運用状況,” IPSJ Magazine Vol.55 No.8 pp.786-793, 2014. (In Japanese)

(2) Conference Papers

4. 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.
5. Atsuya Uno, Hajime Hida, Fumio Inoue, Naoki Ikeda,Toshiyuki Tsukamoto, Fumichika Sueyasu, Satoshi Matsushita, Fumiyoshi Shoji, “Operation of the K computer Focusing on System Power Consumption,” HPCS2015, 2015, Japan. (In Japanese) (to appear)

(3) Invited Talks

- None

(4) Posters and Presentations

3. Keiji Yamamoto, Atsuya Uno, Ryuichi Sekizawa, Daisuke Wakabayashi, Fumiyoshi Shoji, “区間スケジューリングを用いたジョブスケジューリングの性能評価,” IPSJ-SIGHPC 2014-HPC-146 No.3, 2014. (In Japanese)
4. Fumio Inoue, Atsuya Uno, Toshiyuki Tsukamoto, Satoshi Matsushita, Fumichika Sueyasu, Naoki Ikeda, Hajime Hida, Fumiyoshi Shoji, “電力消費量の上限を考慮した「京」の運用,” IPSJ-SIGHPC 2014-HPC-146 No.4, 2014. (In Japanese)
5. Atsuya Uno, Hajime Hida, Naoki Ikeda, Fumio Inoue, Toshiyuki Tsukamoto, Fumichika Sueyasu, Fumiyoshi Shoji, “「京」におけるジョブ単位の消費電力推定の検討,” IPSJ-SIGHPC 2014-HPC-147 No.20, 2014. (In Japanese)
6. Keiji Yamamoto, Atsuya Uno, Ryuichi Sekizawa, Daisuke Wakabayashi, Fumiyoshi Shoji, “区間ジョブスケジューリング法へのファイルステージング導入に伴う性能評価,” IPSJ-SIGHPC 2015-HPC-148 No.29, 2015. (In Japanese)

(5) Patents and Deliverables

- None

Software Development Team

1. Team members

Kazuo Minami (Team Head)
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2. Research Activities

In FY2014, our work focused on the following three areas: (1) activities regarding system operations, (2) analyses of relationship between power consumption and application performance, and (3) performance tuning of several applications.

For system operations, we provided a user support service called the K support desk at which any queries from users were resolved. We also checked if a revised language environment did not degrade or not after it was updated.

Some user applications consumed huge amounts of electric power that exceeded contractual power supply limits. Therefore, we examined relationship between performance characteristics of the applications and corresponding electric power consumption. In addition, we studied a feasibility of an automatic acquisition environment for performance characteristics of user jobs.

As for our efforts regarding performance tuning, we focused on five themes. First, we evaluated and improved the HPCG benchmark on the K computer; note that in November 2014, the K computer was ranked the 2nd place in the list of HPCG BoF at the Supercomputing Conference 2014 (SC'14). Second, we evaluated the computational performance of PHASE that is a first-principles molecular dynamics simulator for nanomaterial software developed by National Institute for Materials Science (NIMS). Third, we upgraded the K-scope, which is a source code analysis tool, as it has a new function of visualizing program structure of C source code in addition to Fortran. Fourth, we performed a study how to summarize tuning history applied to application programs in collaboration with the HPC Usability Research Team of RIKEN AICS. Lastly, we measured the performance of major communication functions of the MPI library for the K computer via a benchmark program.

3. Research Results and Achievements

3.1. Operations of the K computer

3.1.1 User support

We provided user support services named K support desk in collaboration with the system operations and development team. The K support desk has a role of solving any kinds of queries from users, which come from both RIKEN AICS users and general users indirectly via the Research Organization for Information Science and Technology (RIST). RIST is an official organization which is engaged in consultation services for the K computer general users.

We accepted 793 technical inquiries, requests, and problem reports on compilers, profilers, programming support tools, debuggers, numerical libraries, an MPI library, user manuals, and tutorial documents in FY2014. We held a weekly meeting for checking progress on studying them.

We also had 8 meetings with RIST in FY2014 to discuss several issues on user support and give suggestions on techniques for shortening execution time of user applications including methods for identifying tuning spots.

3.1.2 Checking system performance

When system software such as operating systems, compilers, and libraries is updated, we have to check if the update gives any side effects to execution of applications or not. Therefore, we have made routinely a comprehensive checking procedure for computational performance at the end of all system maintenance by using a check suite comprising kernel parts of some user applications.

We had four consecutive updates of language environments in FY2014, which are K-1.2.0-16-2, K-1.2.0-16-3, K-1.2.0-17, and K-1.2.0-17-2. According to checking them by using the check suite, we detected side effects in language environment versions K-1.2.0-16-2, K-1.2.0-16-3 and K-1.2.0-17. As results of our findings, K-1.2.0-16-2 and K-1.2.0-16-3 were released under some limited conditions and K-1.2.0-17 was not formally released at all. As K-1.2.0-17-2 was not detected severe side effects, it was then formally released to all users.

3.1.3 Study on run-time fluctuations

Fluctuations of application run-times disturb efficient operations of the K computer. Fluctuation means the difference of run-time of an application which is found by some reasons on the system, despite the application is carried out in the same execution condition and the same manner. Therefore, we have to study run-time fluctuations and solve them.

In FY2014, we encountered an application having a large run-time fluctuation. Its usual run-time of a certain part of the application is approximately 0.006 seconds, but it sometimes increased to approximately 10 seconds. We found that two factors contributed the fluctuations. One was an asynchronous I/O problem and this gave the application the run-time fluctuation frequently and

largely, which was already known in the previous study. We gave the application user information on avoiding the negative effect of the asynchronous I/O.

The other factor was that it might be derived from a operating system behavior. We just found that the number of instructions ware increased significantly, but we did not solve this problem. We are examining this problem.

3.2 Analysis of the relationship between power consumption and application performance

In high-performance computing, an increase of power consumption along with the advancement of system performance becomes a major concern. We had expected that there were no applications but the LINPACK benchmark program which used almost all parts of the K computer and exceeded power consumption limits. However, we found the cases that power consumption of some applications exceeded such limits by huge-size job executions occupying the entire system of the K computer due to advances of massively parallel coding.

In the operation of the entire AICS facility, the maximum power consumption is limited to 17.75 megawatts (MW), which is the sum of both the electric power amount contracted with the electric power company and the amount generated by the individual co-generation system. If the power consumption exceeds this limit, we temporarily need to be supplied with power beyond that of the value contracted with the power company and paid a financial penalty to them.

Therefore, we have to analyze the relationship between power consumption and application performance.

3.2.1 Measurements of electric power consumption of a user application

We measured a history of consumed electric power of a user application Real-Space Density Functional Theory (RSDFT) in both every 1 second and every100 milliseconds (msec). By every 1 sec measurement, we found that there are the periods in which the electric power consumption was extremely large and DGEMM routine was executed frequently at the period in the diagonalization (DIAG in Fig. 1) and the orthogonalization (Gram–Schmidt in Fig. 1) of the matrix. The downward spikes within the periods in Fig. 1 represent inter-node communications. Measurements at 100 msec intervals revealed that intensive memory access consumed huge amounts of electric power.

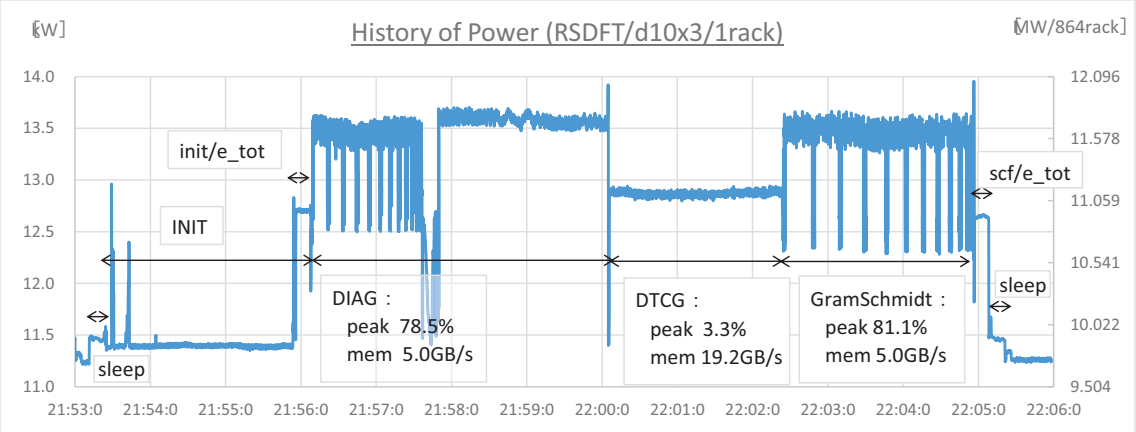

Figure 1 History of electric power consumption

3.2.2 Consideration on the relationship

Power consumption can be evaluated by associating the characteristics of application performance, such as the efficiencies of floating-point calculation performance, main memory throughput, L2 cache throughput, L1 data cache throughput, and integer calculation performance. These characteristics can indicate application performance by measuring the run-time of an application.

We measured power consumption using some loop collections that comprised basic operations. As a result, we established the relationship between power consumption and the evaluation characteristics by the following equation,

$$\begin{aligned}\text{Power consumption[MW/sys]} &= 1.3659 \times \text{Floating Calc.[\%]} \\ &+ 4.3906 \times \text{Main memory throughput[\%]} + 0.0857 \times \text{L2 cache throughput[\%]} \\ &+ 2.3299 \times \text{L1D cache throughput[\%]} + 0.2429 \times \text{Integer Calc.[\%]}\end{aligned}$$

We found that main memory throughput has greater influence on power consumption than floating-point calculations. Figure 2 shows a comparison between the measured values and the estimated values for power consumption based on the equation.

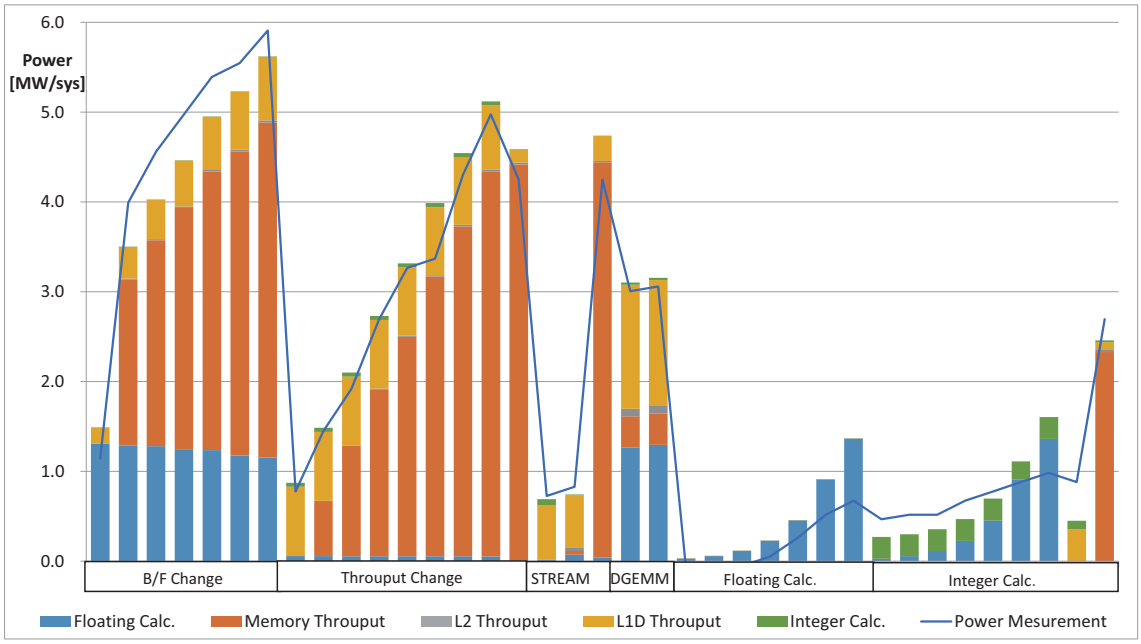

Figure 2 Comparison between measured and estimated power consumption

As shown in Fig. 3, the power consumption of loops which was extracted from real applications was compared to the estimated value by the eqauation. As indicated in the figure, we found that the power consumption of loops in actual applications was able to be explained by using an evaluation of the basic loop.

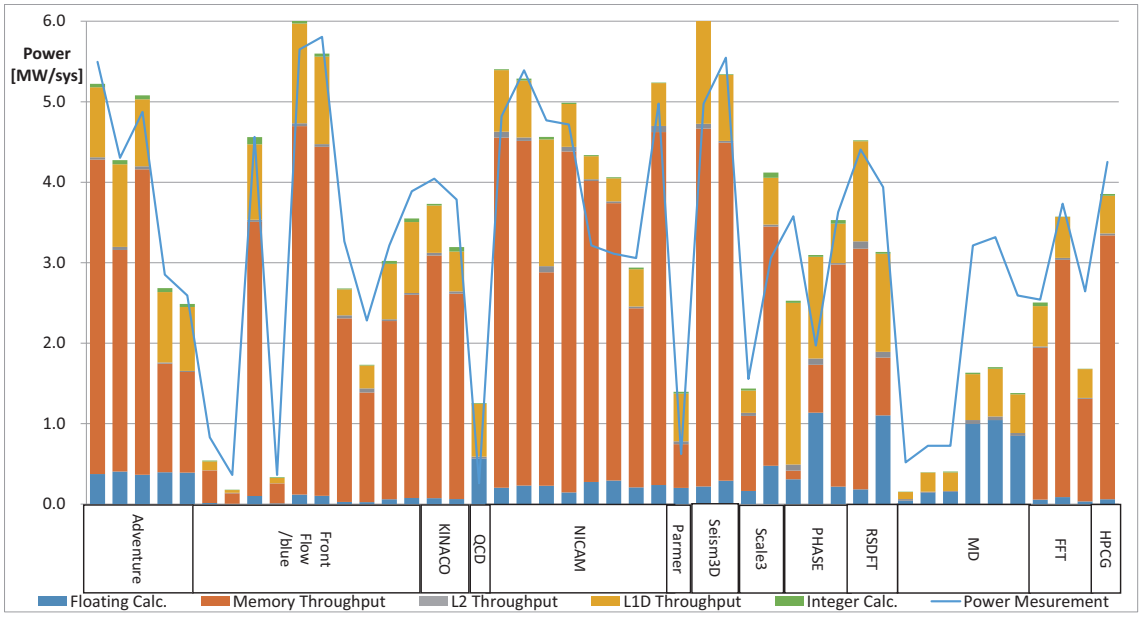

Figure 3 Comparison of measured power consumption of applications and the estimated values

3.2.3 An analysis of large power consumption of applications

In February 2014, the power consumption of the entire AICS reached 19.3 MW. We found that an application which used all nodes of the K computer by flat-MPI execution assigning 8 MPI processes to each node caused this excess beyond the upper limit.

To determine this, we built a special environment in which power consumption of the application can be measured. And investigations of this application ware carried out under several conditions. As a result, we found flat-MPI execution required large memory access by the two reasons; (1) Inter-process communication within a node is performed via memory copies and (2) the effective L2 cache memory size per process becomes smaller because L2 cache memory is shared by multiple processes within a node. As mentioned in Section 3.2.2, memory access gives a significant impact on power consumption. Therefore, flat-MPI applications require large power consumption.

In addition, we found large power consumption at calling the MPI_Finalize function, because the MPI_Finalize functions invoke memory accesses in proportion to the square of the MPI processes and therefore the number of memory accesses increased. We measured the power consumption of the MPI_Finalize function in flat-MPI coding under several conditions, and found that the power consumption for a rack reached 5.52 kW with 144 computer racks in which 110.592 MPI processes. Therefore, we estimated the maximum number of processes to be approximately 530,000 processes for flat-MPI in order that the power consumption increase is within 3.8 MW. Moreover, by a constraint that running time of flat-MPI program should be less than 15 minutes, the maximum number of MPI processes should be approximately 300,000 processes. From the viewpoint of practical use, the maximum number of processes of flat-MPI should be smaller than these numbers.

3.2.4 Automatic acquisition environment for computational characteristics of user jobs

A user application program is characterized by utilization load balancing among such computer system parts as the arithmetic unit, memory, inter-node communication, and disk I/O.

Although almost all user applications impose a load concentrated on any one of these computer system parts, some user applications never impose a significant load at all and does not use computer resources efficiently. Tuning of such the applications is a valid approach to more effectively utilizing computer resources.

Therefore, we studied an acquisition tool which obtains automatically load characteristics of each user job and found the tool was feasible. For example, the accounting PA function is able to collect the number of floating-point operations (FLOP count) and memory throughput of each user job. By the combination of information both from the accounting PA function and from the Tofu-sar function, we are able to collect the number of inter-node communications and the amount of inter-node communications for each user job.

We plan to construct such an automated environment and start collecting user job characteristics information early in FY2015.

3.3 Performance tuning

3.3.1 HPCG

The LINPACK benchmark has long been used as a performance metric for supercomputers, however, there are some opinions that LINPACK is biased to measure computational performance and is no longer a realistic metric. Recently, the high performance conjugate gradient benchmark program (HPCG) has been proposed as an alternative metric for supercomputers in the International Supercomputing Conference held in 2014. HPCG measures the speed of solving symmetric sparse linear system equations using the conjugate gradient method with a multi-grid symmetric Gauss–Seidel smoother.

We evaluated and improved the performance of HPCG on the K computer using an early version prior to its official announcement. Weak scaling measurements of HPCG on the K computer had good parallel scalability; however, its single CPU performance was very low. We therefore tuned single CPU performance. Since runtime is primarily consumed by two kernels performing matrix and vector multiplication, we tuned in the following areas: (1) memory layout improvement; (2) data access ordering improvement; (3) multi-threading, especially for indirect memory accesses; (4) loop optimization; and (5) running parameter adjustments.

As a result, we achieved a speed approximately 19-times greater than the original. In November 2014, the K computer marked 0.461 PFLOPS using 82,944 nodes and ranked the 2nd in the list of HPCG BoF at SC'14. Note that this rank was higher than that of the Titan supercomputer at Oak Ridge National Laboratory, though the Titan has a higher LINPACK score than the K computer.

3.3.2 K-scope: source code analysis tool

K-scope is a source code analysis tool that visualizes program structure in the form of a tree to give uses some hints of bottleneck candidates, including loops, branches, and procedure calls; the tool is useful for researchers and tuning experts aiming to improve application performance. We have distributed this tool since FY2012 as part of the AICS software.

In FY2014, as an experimental study, we collaborated with Kobe University and the RIKEN AICS research team to develop new K-scope features, including the following:

1. A basic design for visualization of C source code program structure

K-scope uses a front-end program of the Omni XcalableMP compiler (XMP) as a translator that converts Fortran code into intermediate code. In FY2014, we devoted a feasibility study to visualizing program structure of C source code using intermediate code created by a front-end of

XMP. From this study, we learned that K-scope can visualize the program structure of C source code using intermediate code as with Fortran; however, to enhance the analysis features for C source code, we found the need to further revamp XMP.

2. Development of an Eclipse plug-in to visualize program structure

While the latest version of K-scope can visualize program structure by itself, it offloads editing features to an external editor. In general software development aside from HPC, most developers use an integrated development environment (IDE) along a workflow that includes editing, compiling, and debugging. In FY2014, we collaborated on an experimental study with Yokokawa laboratory in Kobe University and implemented new features as an Eclipse plug-in to visualize program structure in the form of a tree. With this deliverable, a user can visualize the program structure within the Eclipse framework. Also, we concluded an agreement for the mutual use of the intellectual property obtained via this collaboration.

3.3.3 A study of tuning history for the enhancement of a tuning environment

Performance improvements for an application comprises two steps; finding a bottleneck using profilers, then rewriting the source code. This is a form of engineering; however, such performance is strongly influenced by the rewriting of source code. Therefore, we are able to use an ad-hoc solution instead of engineering with sufficient investigation. However, even if we have tips and know-how regarding performance optimizations for an application, it is difficult to marshal this knowledge systematically and reuse it for another similar application.

Based on our empirical knowledge, tuning methods for performance improvement (which appear in typical textbooks), such as loop unrolling, loop fission, and loop fusion, are often used; however, there is no organized database to investigate the relationship between rewriting code and resulting performance. Therefore, to collect actual tuning cases, we created tuning histories based on our previous work in performance improvement. Also, to assess the impact rewriting code has on performance, we created micro-benchmarks, which comprise various loop transformations. To easily estimate the relationship between code and performance, their tuning histories and micro-benchmarks comprise source code with profiling results. In FY2014, this study was conducted by collaboration with the HPC Usability Research Team in RIKEN AICS.

3.3.4 Measurement of MPI performance

We measured the performance of major communication functions in the MPI library by using a benchmark program and developed an environment to compare results with those measured in the past. More specifically, we measured the performance of sixteen communication functions specified in the MPI version 1, including both collective communication functions (e.g., MPI_Allreduce,

MPI_Bcast) and point-to-point communication functions. Measurements were performed across nine cases in total and covered three groups of computer nodes; Each group comprised 384, 3072, and 18,432 nodes. Furthermore, three kinds of node allocation, namely one-, two-, and three-dimensional allocation were used in the measurements.

Performance of MPI_Bcast function reached 10 GB/s when computer nodes were allocated in three dimensions. Performance of MPI_Allreduce also reached 6 GB/s, when an option of static work area allocation was enabled.

3.3.4 PHASE

We tuned and measured the detailed performance of the density functional theory first-principles calculation application PHASE. The target problem was the analysis of a wide-gap semiconductor SiC-SiO_2 interface. A large amount of parallelism is required to calculate given the limitations of elapsed time and memory size, because the elapsed time and memory size of the application increases with the cubic square of the number of atoms in the density functional theory.

In general, we need Fourier transforms to use the reciprocal space, which is one way to expand the wave function. All-to-all MPI communications are also required for transposition of data axis and generally not suitable for massively parallel systems. Therefore, in this study, we developed multi-dimensional parallelization to solve these problems. As a result, high scalability was achieved by confining all-to-all MPI communications in small regions of processors, and the peak performance was also improved since the loop length became large.

In addition, we applied process mapping for two sub-communicators of all-to-all MPI communication to optimize the Tofu algorithm for improving performance of the biaxial distributed three-dimensional FFT. We achieved a peak performance of 21.2% (2.25PF), including FFT in the calculation, which is a wide-gap semiconductor SiC-SiO_2 interface of 25,200 atoms using a full 82,944 nodes on the K computer. We also achieved strong scalability of approximately 1,728 times in the calculation of 3,848 atoms using from 48 to 82,944 full nodes on the K computer.

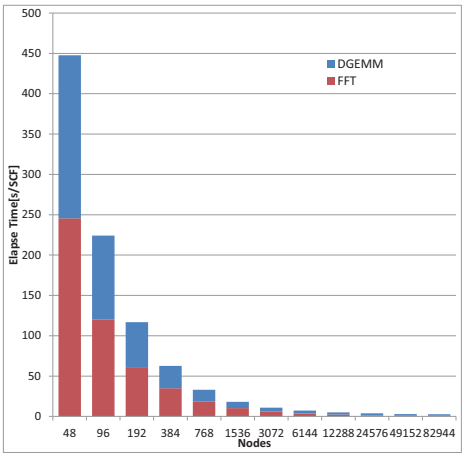

Figure 4 Strong scalability for SCF calculation in PHASE

The calculation time was reduced from 441 seconds to 2.81 using 48 nodes for a self-consistent field (SCF) calculation. This calculation speed corresponds to a reduction from about 51-day simulation to 8 hours for the structural relaxation calculations. This signifies that a long relaxation simulation using the number of parallelism much larger than the number of atoms is possible.

4. Publications, Presentations, and Deliverables

(1) Conference Papers

1. Masaaki Terai, Peter Bryzgalov, Toshiyuki Maeda and Kazuo Minami, “Extending K-scope Fortran Source Code Analyzer with Visualization of Performance Profiling Data and Remote Parsing of Source Code,” The 6th International Symposium on Advances of High Performance Computing and Networking (AHPCN) within International Conference on High Performance Computing and Communications (HPCC-2014), pp. 878–885, (2014).

(2) Invited Talks

1. Kiyoshi Kumahata, Kazuo Minami, Naoya Maruyama, HPCG on the K computer, ASCR HPCG WORKSHOP, (https://www.orau.gov/hpcg2014/presentations.htm).
2. Kiyoshi Kumahata, HPCG Performance Improvement on the K computer, HPCG BoF at SC14, (http://www.hpcg-benchmark.org/custom/index.html?lid=154&slid=271).
3. Kazuo Minami, Overview of the new benchmark HPCG and its performance on the K computer (in Japanese), The Society of Scientific Systems, HPC forum 2014, (http://www.ssken.gr.jp/MAINSITE/event/2014/20140826-hpcf/index.html).
4. Kazuo Minami, Kiyoshi Kumahata, Naoya Maruyama, HPCG Performance Improvement on the K computer, Proceedings of the 21th Workshop on Sustained Simulation Performance (WSSP), pp.191-206, 2014, (https://www.sc.isc.tohoku.ac.jp/wssp21/index.en.html).

5. Kiyoshi Kumahata, HPCG performance improvement on the K computer, The 65th AICS Cafe, 2014, (http://aics-research.riken.jp/cafe.html).

(3) Posters and presentations

1. Masaaki Terai, Hisashi Yashiro, Kiyotaka Sakamoto, Shin-ichi Iga, Hirofumi Tomita, Masaki Satoh and Kazuo Minami, “Performance Optimization and Evaluation of Global Climate Application using 440m Horizontal Mesh on the K computer,” The International Conference for High Performance Computing, Networking, Storage and Analysis (SC14), (2014).

(4) Patents and Deliverables

1. K-scope: Fortran source code analysis tool (http://www.aics.riken.jp/ungi/soft/kscope/).

HPCI System Development Team

1. Team members

Manabu Hirakawa (Team Head)
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Osamu Tatebe (Visiting Scientist)
Manabu Higashida (Visiting Scientist)
Akira Kondo (Technical Staff)
Koichiro Ozaki (Technical Staff)
Hidetomo Kaneyama (Technical Staff)
Satomi Yasuda (Assistant)

2. Research Activities

We are involved in technical development of an innovative high performance computing infrastructure (HPCI) that will connect the major Japanese supercomputers installed in universities and research institutes, including the K computer, through a network. The computing environment realized by the HPCI will meet the diverse needs of its intended users. Furthermore, the high-speed network will enable the supercomputers, shared storage, and other functionalities of each HPCI system provider to operate as a common HPCI. To this end, we are working on the technical side of the entire system operation, the technical coordination of the facilities comprising the HPCI system, and the operation of HPCI Shared Storage (HPCI-SS).

The HPCI-SS is a large-scale distributed file system comprising 4 meta-data and 40 file-data servers. The HPCI-SS forms the data-sharing infrastructure of the HPCI led by the Ministry of Education, Culture, Sports, Science and Technology (MEXT). It provides a 22 PB single-view "Gfarm" network file system that is open to all HPCI users and supports scalable I/O performance in a geographically widely distributed environment. In fact, the HPCI-SS meta-data servers are located in RIKEN AICS and the University of Tokyo (U-Tokyo), while the file-data servers are located in AICS, U-Tokyo, and the Tokyo Institute of Technology (Tokyo Tech). HPCI-SS also supports single sign-on authentication (GSI-AUTH), by which users can exchange their computational results between their local storage systems and HPCI-SS without additional authentication.

HPCI-SS has developed into a key infrastructure for the management and sharing of computational data in HPCI projects.

3. Research Results and Achievements

3.1. HPCI Shared Storage System

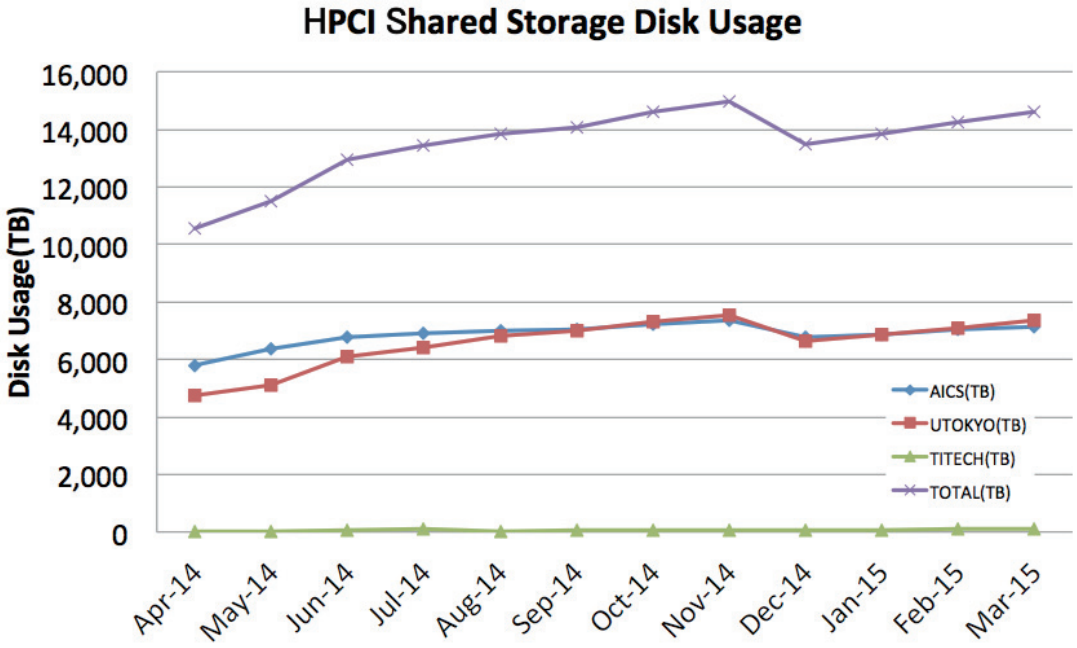


Figure 1 Disk usages of HPCI-SS

Figure 1 shows the disk usage of HPCI-SS in FY2014. Disk usage increased almost monotonically, reaching 14.61 PB (65%) at the end of FY2014. If this rate continues, the disk space of the HPCI-SS will become exhausted in FY2015.

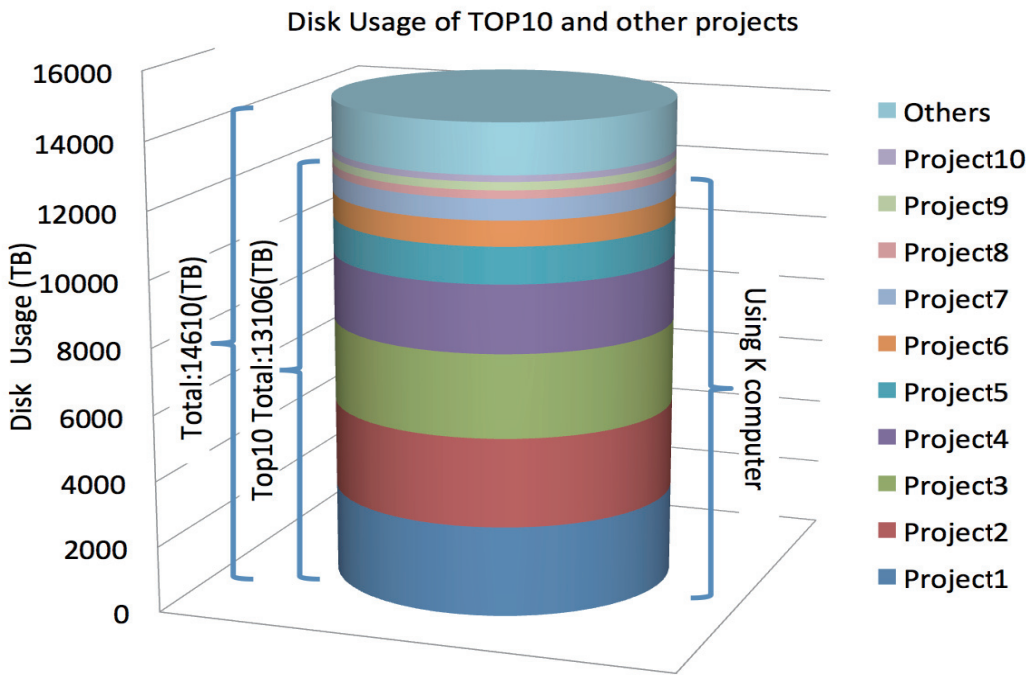
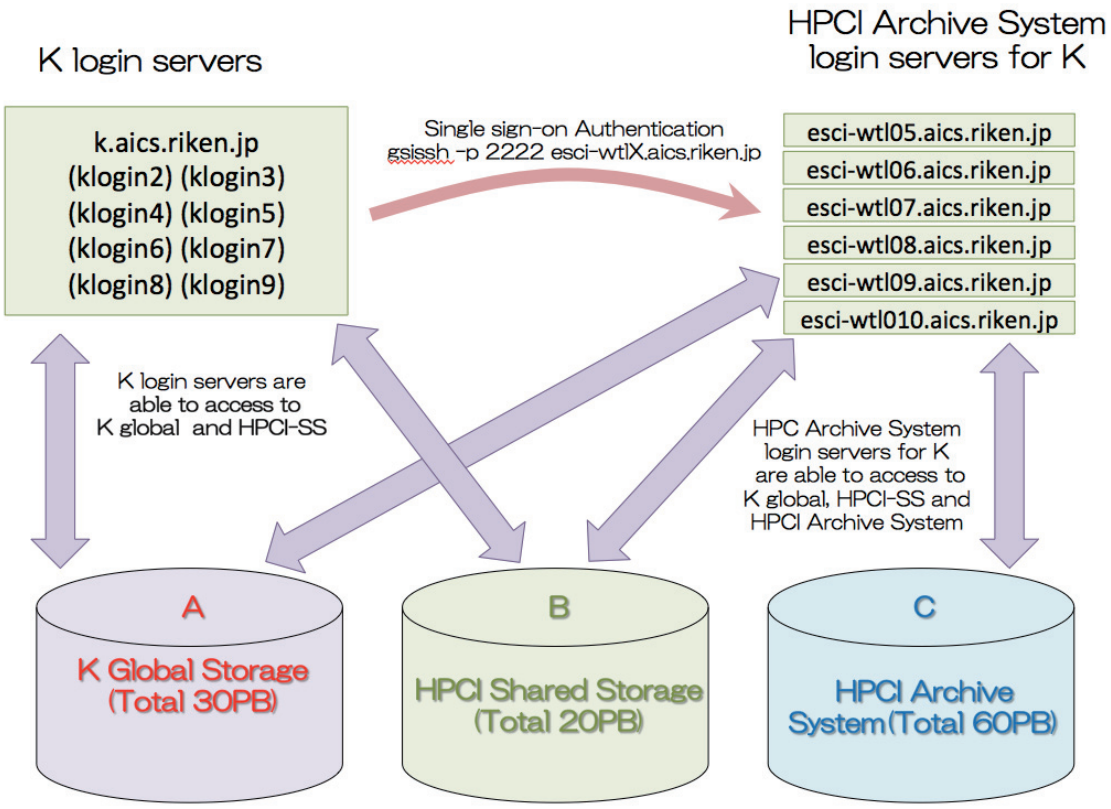


Figure 2 Disk usage of the top 10 HPCI projects

In FY2014, HPCI-SS access was granted to 44 HPCI research projects. Figure 2 shows the disk space consumed by the top 10 HPCI projects in March 2015. The top 10 projects occupy 89.7% of the total disk usage and 8 of these projects use the K computer. To avoid exhausting the disk space, an accessible archive space for users of the K computer is urgently required.

3.2. Archive System for Users of the K Computer

As a backup environment of the HPCI-SS disk resource, we constructed the tape HPCI Archive System (HPCI-AS) login server for K computer users at the end of FY2014.



The standard HPCI-AS login servers allow HPCI users to access the HPCI-AS file system, but allow no access to K's Global File System (GFS). Therefore, K users could not directly transfer their computational data from GFS to HPCI-AS.

Subsequently, the HPCI system development team constructed special HPCI-AS login servers through which K users can copy their data. These special login servers statically mount the GFS, including the home and data area of the K computer. Within this environment, K users can access and directly transfer data among three file systems; GFS, HPCI-SS, and HPCI Archive. To enable access to GFS, the local account of a K user's HPCI-AS login server matches his or her local K computer account and GFS client packages are installed by FUJITSU.

At the end of FY2014, the user accounts of 524 K computer users involved in 32 research projects were registered in these login servers.

3.3. Long-term data archive project

The Research Organization for Information Science and Technology (RIST) requested that the computational data of expired research projects be archived in HPCI-AS for three years. Complying with this request, 119 TB of the computational data of five expired projects were archived in FY2014 and will be saved until the end of FY2016.

3.4 Data Analyzer Servers

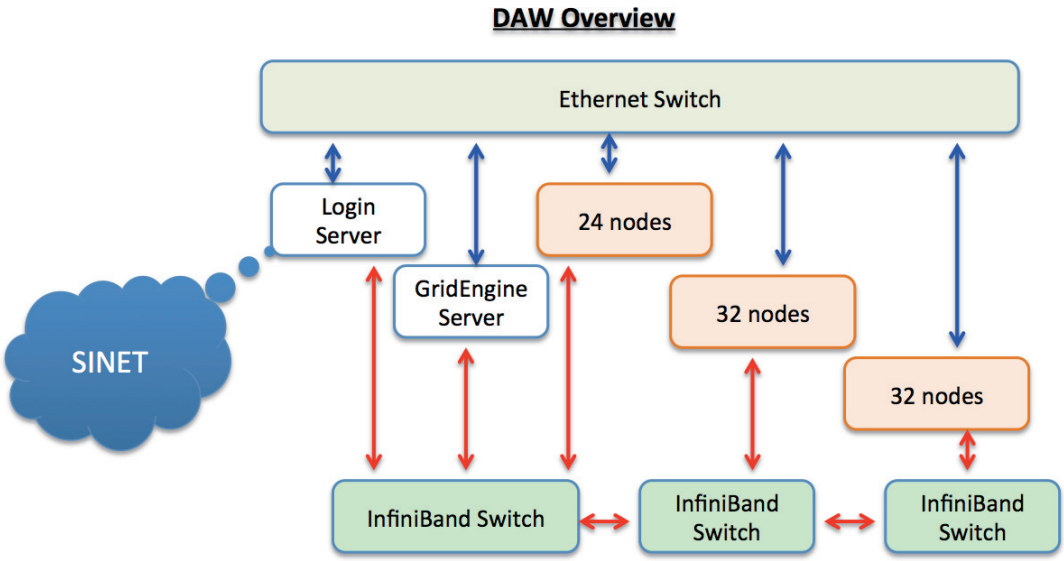


Figure 3 Overview of data analyzer west

Another HPCI computational resource is the 88-node linux cluster called "Data Analyzer West (DAW)." As shown in Figure 3, the 88 computational nodes and 2 servers of DAW are connected by an InfiniBand network. An Intel compiler, OpenMPI, mvapich2, and GridEngine job scheduler are also available in the DAW environment.

In FY2014, this cluster machine was made available to three HPCI research projects. Figure 4 plots the monthly execution node-time occupied by each project.

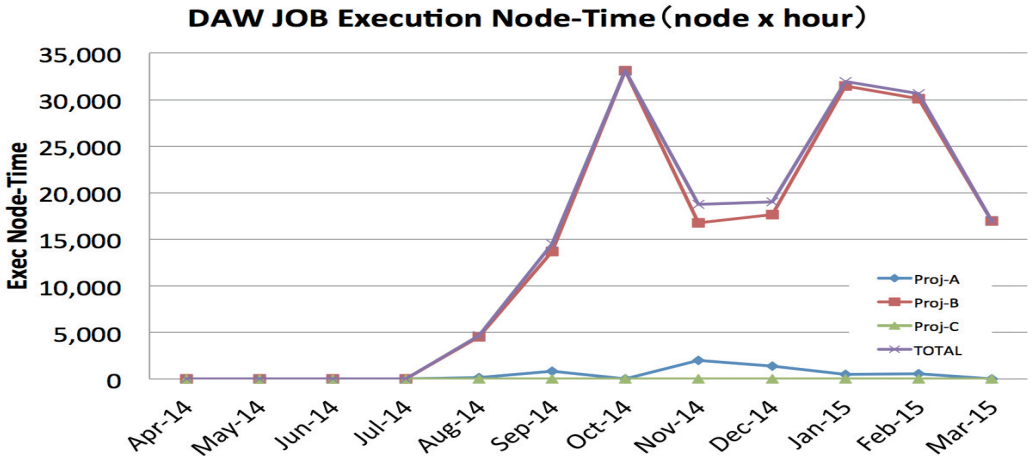


Figure 4 Node-hour usage of data analyzer west

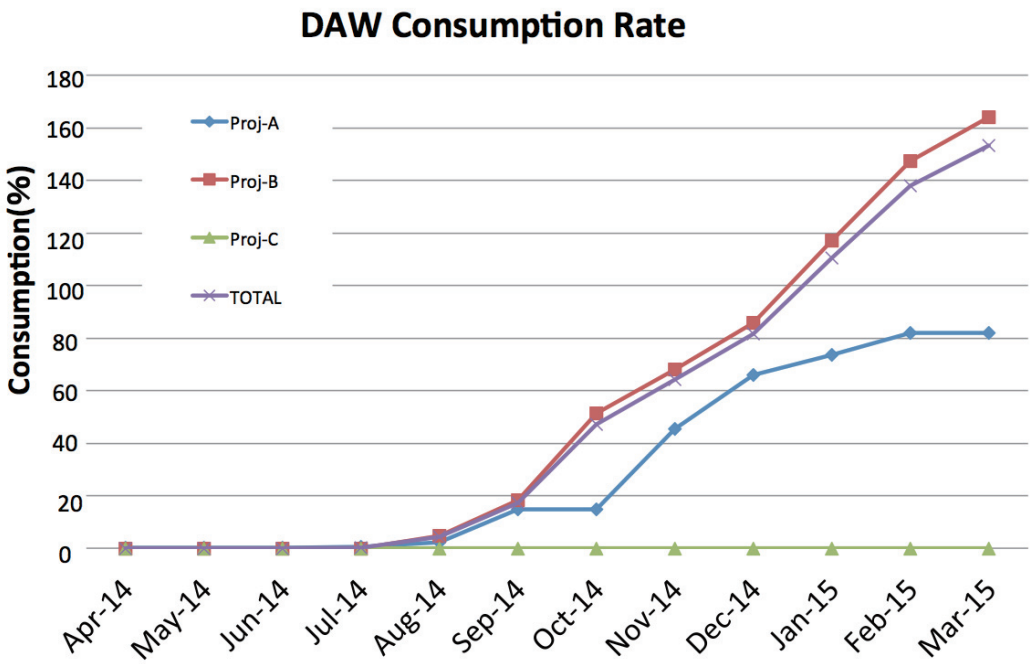


Figure 5 Consumption rate of projects using the DAW cluster machine

Figure 5 plots the monthly node-time consumption rate of each project. The three projects collectively consumed 153% of the allocated node-time.

3.5 User Support

Cooperating with the U-Tokyo and Tokyo Tech teams, the HPCI System Development Team has developed user supports such as HPCI user management and Gfarm consulting services.

- Four HPCI projects and 600 or more scientists were using HPCI-SS at the end of FY2014. User support is provided through the HPCI Help desk and the hpci-tech@aics.riken.jp mailing list.
- Technical information on the HPCI-SS and HPCI-AS, including the system configuration, manuals, tips, services, and maintenance schedules, are available through the HPCI CMS web site.
- The HPCI-SS usage of each project is conveyed to project leaders through our monthly reports.
- Technical consulting service on HPCI-SS is provided by Prof. Tatebe, U-Tokyo, and Tokyo Tech.

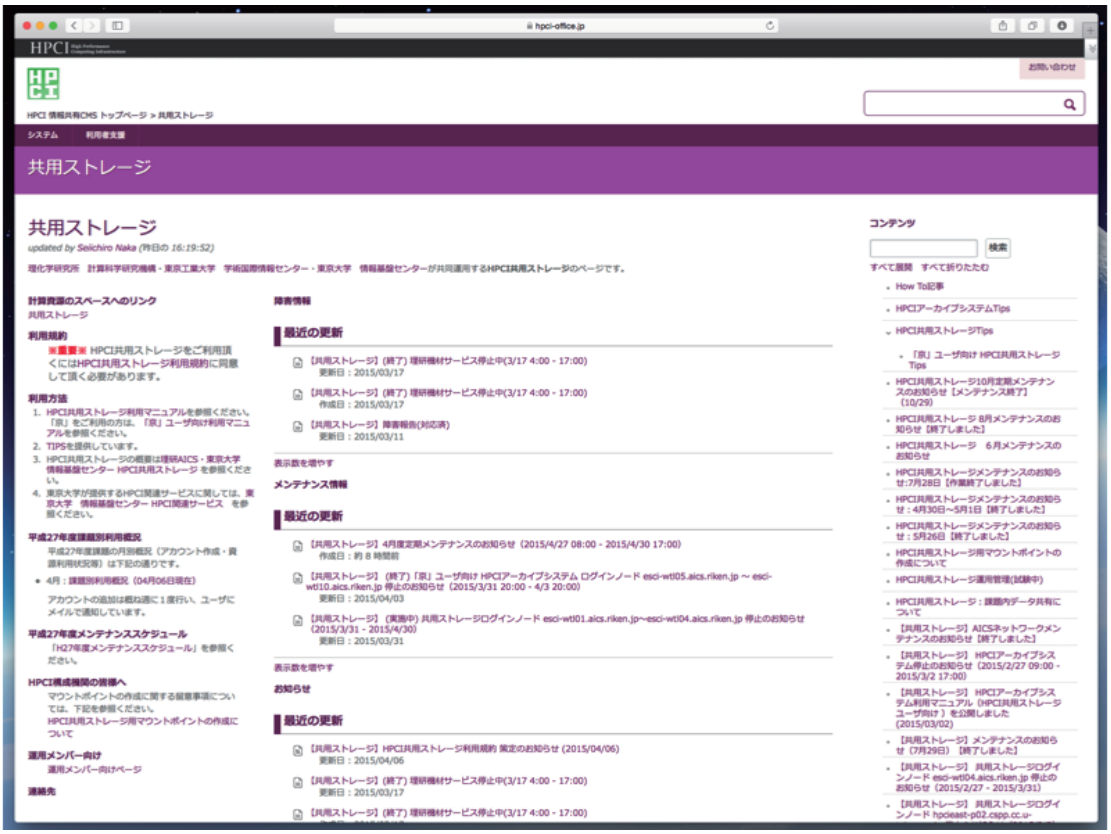


Figure 6 Web page for user support

3.6 Technical Coordination

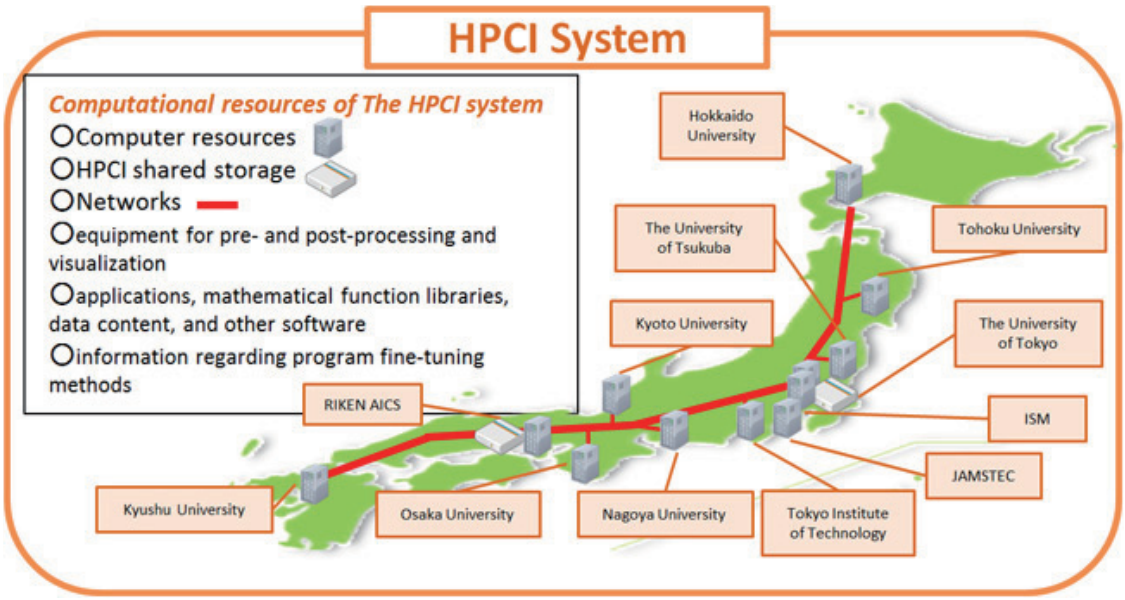


Figure 7 Overview of HPCI

As shown in Figure 7, computational resources for the HPCI system are provided by the supercomputer centers of nine universities, RIKEN AICS and the Japan Agency for Marine-Earth Science and Technology (JAMSTEC). The Institute of Statistical Mathematics (ISM) has provided its resources since July 2014.

- HPCI System Monitoring

HPCI system monitoring enables us to monitor the status of the computing resources provided by each HPCI system provider, the operational status of the network, and the bandwidth and throughput performance. The HPCI system monitoring performs the following roles:

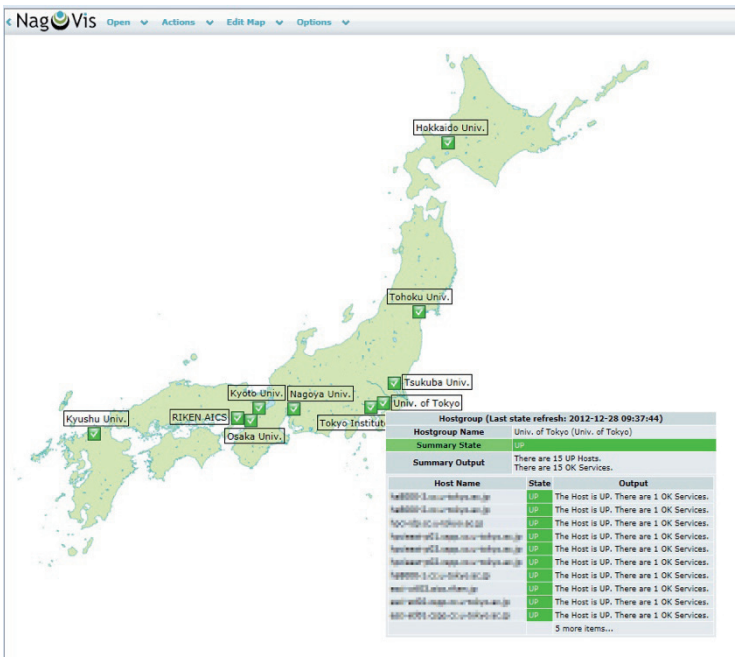


Figure 8 Overall monitoring system - Nagios/Nagvis

- Coordinates and manages meetings for HPCI system providers and other relevant bodies
  - Hosted meetings of the HPCI Cooperation Service Committee (3 times)
  - Hosted meetings of the HPCI Cooperation Service and Operation Working group (11 times)
  - Hosted meetings of the HPCI Shared Storage Operation team (11 times)
- Investigates the causes and response measures of technical problems that occur during the operation of the HPCI system
- Researches the improvement of software related to the operation of the overall HPCI system
- Operates and maintains the HPCI shared storage site (the West site)
- Operates and maintains the management of Login Gateway and the HPCI IdP of AICS (one of the HPCI system providers)

- Develops the HPCI online application system
- Screens institutions seeking to participate in the shared operation (i.e., seeking to provide computing resources to the HPCI system) to check whether they satisfy the technical requirements.

4. Schedule and Future Plan

As mentioned above, if the disk space usage increases at the current pace, the HPCI-SS disk space will become exhausted during FY2015. As a preventative measure, we will encourage use of the HPCI-AS by improving the performance of file transfer to HPCI-AS. To this end, we will adapt the Gfarm parallel file copy command “gfpcopy.”

In FY2015, five or six long-term system maintenances are scheduled by U-Tokyo and AICS.
The new version of Gfarm (version 2.6) was released in March 2015 and the user-level transparent meta-data server failover is now implemented. By virtue of its failover functionality, the Gfarm meta-data server is expected to effectively minimize interference by system maintenance at the site level. For this purpose, AICS and U-Tokyo will construct a mutual failover relationship between each meta-data server. This relationship will maintain the HPCI-SS system operational even during system maintenance at U-Tokyo or AICS.

The FY2015 HPCI research projects are already published and three projects have been accepted for access to DAW. The total allocated node-time is approximately 40% of DAW’s capacity. Most of the computational nodes are expected to remain idle, with consequent wastage of electric power. To reduce DAW’s power consumption, we will introduce an automatic idling stop operation to DAW’s computational nodes in early FY2015, which will automatically shut down any idle nodes. When jobs requiring more nodes enter the scheduler queue, these down-state nodes will be booted up and available for executing the jobs.

5. Publication, Presentation and Deliverables

(1) Conference Paper

1. 實本,塙,原田,中,建部,平川,藤本,蛯原,宮嵜,佐島,”HPCI ストレージの運用,” AXIES 大学 ICT 推進協議会年次大会,Dec2014

(2) Presentation

1. 原田,”HPCI 共用ストレージの歩み-『革新的ハイパフォーマンス・コンピューティング・インフラ』におけるデータ共有基盤として,”Gfarm シンポジウム 2014,Dec2014

(3) Manuals

1. ”HPCI 共用ストレージ利用マニュアル「京」ユーザ向け,”Dec2014
2. ”HPCI アーカイブシステム利用マニュアル「京」ユーザ向け,”Dec2014
3. ”HPCI アーカイブシステム利用マニュアル,”Feb2015

System Software Development Team

1. Team members

Yutaka Ishikawa (Team Leader)
Masamichi Takagi (Senior Research Scientist)
Balazs Gerofi (Research Scientist)
Takahiro Ogura (Research and Development Scientist)
Atsushi Hori (Research Scientist)
Akio Shimada (Research and Development Scientist
Masayuki Hatanaka (Research and Development Scientist)
Norio Yamaguchi (Research and Development Scientist)
Fumiyoshi Shoji (Research and Development Scientist)
Atsuya Uno (Research and Development Scientist)
Toshiyuki Tsukubamo (Research and Development Scientist)
Keiji Yamamoto (Research and Development Scientist)
Toyohisa Kameyama (Technical Staff)

2. Research Activities

Our team mission is to develop the system software stack for the successor of the K supercomputer, called Post K, which will be based on a manycore architecture. The basic design of the software stack shown in Figure 1 has been performed in cooperation with Fujitsu since October of 2014.

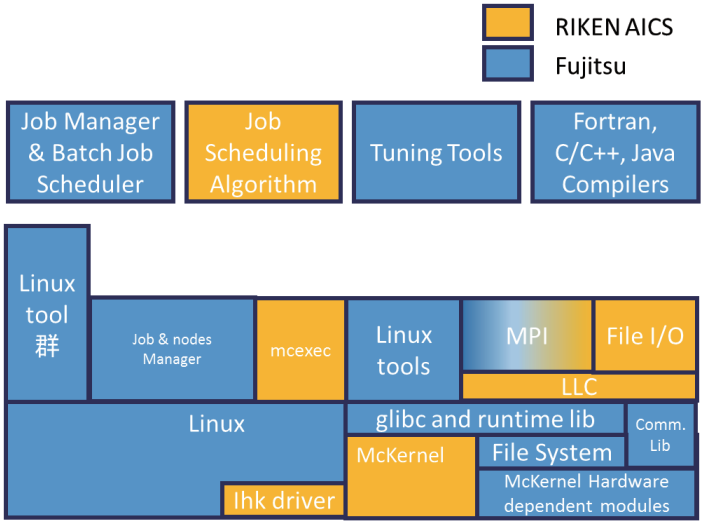


Figure 1 System Software stack

The system software stack, especially developed at RIKEN, is not only designed for Post K, but also designed for other commercial manycore architectures, such as an Intel Xeon phi. The software stack,

we have focused on in FY2014, has an OS kernel, called McKernel, a lowlevel communication library, called LLC, and file IO library. At the same time of designing the software stack, we have studied on parallelization of one of the representative target applications, called Genomon. The research progress on McKernel and Genomon parallelization is reported below.

3. Research Results and Achievements

3.1. McKernel

McKernel was originally developed at the University of Tokyo. The development is taken over by System Software Development Team. In FY2014, we specified the McKernel version 1.0 feature and we cleaned up the McKernel codes, fixed bugs, and implemented a part of version 1.0 features.

Resource partitioning without modifying Linux Kernel

McKernel needs to divide node resources into at least two partitions, i.e. Linux and the light weight kernel. We eliminate the need for modifying Linux Kernel for the partitioning by creating a Linux kernel module that performs it using CPU hotplug functionality of Linux.

Linux-compatible memory management for physical pages of processes running on McKernel

A process running on McKernel reuses a kernel module running on Linux. The kernel module needs to modify the property of a physical page of the process, i.e. incrementing its reference counter to preventing it from getting paged-out. We developed a memory-management mechanism to allow the kernel module to perform such a modification.

Linux-compatible system calls

We continued implementing system calls. The implementation is validated using Linux Test Project (LTP) test programs and all but one of 1013 tests passes.

Linux-compatible procfs/sysfs

procfs/sysfs is a special file system which provide access to the system properties. The entries are explicitly added by kernel-modules and call-back functions that are called when access to them are registered at that time. Some entries are associated with properties of Linux running on a Linux partition and others McKernel. We choose to reuse as many entries provided by Linux running on a Linux partition as possible by redirecting accesses to entries to the McKernel-specific entries only when they exist. We performed investigation on the McKernel-specific entries this year, as a preparation for the implementation.

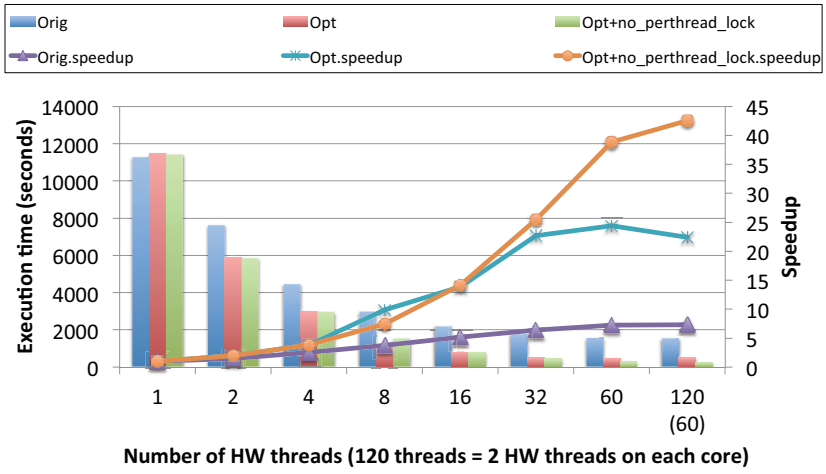
Porting gdb

We have been porting gdb to McKernel. We decided to use a transparent usage model where users can use gdb in a way that they don’t need to know what kind of OS, i.e., Linux or McKernel they are using. The porting is validated using the test programs called “gdb.base” associated with gdb source code and 216 of 312 tests pass so far.

3.2 Genomon

Genomics has been identified as one of the high priority research areas with regards to the development of the postK supercomputer and consequently the GENOMON workflow has been chosen as its representative target application.

GENOMON involves various different tools, from which the most computation intensive component is BLAT. BLAT on DNA is designed to quickly find sequences of 95% and greater similarity of length 25 bases or more. BLAT has been originally designed as a single threaded application and it works by keeping an index of the entire genome in memory. In order to exploit node level parallelism one could run multiple BLAT instances, however, memory consumption quickly becomes a pressing issue.



To overcome this problem, we have parallelized the BLAT code to efficiently exploit symmetric multi-threading. We used OpenMP constructs in conjunction with atomic operations to enable worker threads to update the BLAT data structures in a concurrent fashion. Figure XX shows scalability measurements on an Intel Xeon Phi CPU with up to 120 threads.

4. Schedule and Future Plan

The basic design continues until September of 2015. From October, we will start to develop the whole system software stack. The delivery of the system will start from FY 2018 and after testing and tuning the system, it will be publically operated from FY2020.

5. Publication, Presentation and Deliverables

(1) Journal Papers

(2) Conference Papers

1. Balazs Gerofi, Akio Shimada, Atsushi Hori, Masamichi Takagi, Yutaka Ishikawa , CMCP: a novel page replacement policy for system level hierarchical memory management on many-cores, in Proceedings of HPDC, 2014.
2. Balazs Gerofi, Masamichi Takagi, Yutaka Ishikawa, Exploiting Hidden Non-uniformity of Uniform Memory Access on Manycore CPUs, In Proceedings of Euro-Par Workshops (2), 2014.
3. Taku Shimosawa, Balazs Gerofi, Masamichi Takagi, Gou Nakamura,Tomoki Shirasawa, Yuji Saeki, Masaaki Shimizu, Atsushi Hori, Yutaka Ishikawa, “Interface for Heterogeneous Kernels: A Framework to Enable Hybrid OS Designs targeting High Performance Computing on Manycore Architectures,” IEEE International Conference on High Performance Computing, 2014.

(3) Invited Talks

1. Yutaka Ishikawa, Two Types of Supercomputer Developments, 2014 ATIP Workshop: Japanese Research Toward Next-Generation Extreme Computing, Austin, 17th November 2014.
2. Yutaka Ishikawa, "The Post K Project and Its Big Data Aspect", BDEC (Big Data and Extreme-scale Computing) workshop, Barcelona, 29th-30th January 2015.
3. Yutaka Ishikawa, “Design Consideration for Data Assimilation in Post K Supercomputer”, The 4th International Symposium on Data Assimilation, Kobe, 23rd February 2015.

(4) Posters and presentations

(5) Patents and Deliverables

Architecture Development Team

1. Team members

Mitsuhisa Sato (Team Leader)
Miwako Tsuji (Research Scientist)
Takenori Shimosaka (Research & Development Scientist)
Matsuko Matsusue (Assistant)
Kazuo Minami ((conc.) Research & Development Scientist)
Hitoshi Murai ((conc.) Research Scientist)
Yoshito Kitazawa ((conc.) Research & Development Scientist)
Kiyoshi Kumahata ((conc.) Research & Development Scientist)
Akiyoshi Kuroda ((conc.) Research & Development Scientist)
Kengo Miyamoto ((conc.) Research & Development Scientist)
Fumiyoshi Shoji ((conc.) Research & Development Scientist)
Masaaki Terai ((conc.) Research & Development Scientist)
Yoshiyuki Tsukamoto ((conc.) Research & Development Scientist)
Atsuya Uno ((conc.) Research & Development Scientist)
Yuesu Kodama (Visiting Researcher)
Hitoshi Ukawa (Student Trainee)

2. Research Activities

The architecture development team designs the architecture of post-K computer in cooperation with the vendor partner. The concept of the design is "Co-design", where the system should be designed to support a wide range of scientific applications by taking characteristics of applications into account. In addition to the design of the post-K computer, we are developing performance verification environment to verify the design. And, we also investigated programming environment for the post-K computer.

3. Research Results and Achievements

3.1. Co-Design for Post-K Computer

Since Fujitsu Ltd. had been selected as a partner company in October 2014, we have carried out the basic design for the post-K computer with Fujitsu. The target architecture parameters we have investigated include node architecture, cache, network, memory technologies, and so on. Based on the co-design concept, we have evaluated the performance of target applications by varying various sets of these parameters.

3.2 Performance Evaluation Environment & Tools for Post-K Computer

We are developing performance verification environment to verify the design of the post-K computer. In 2014, we have developed a set of CPU-simulator and compiler for the simulator. For the simulator, gem5 simulator system, which is a modular platform for computer system architecture research, encompassing system-level architecture as well as processor microarchitecture (gem5.org), has been extended to sparc64 viiifx. For the compiler, LLVM compiler, which is a collection of modular and reusable compiler and toolchain technologies (llvm.org), has also been extended to sparc64 viiifx to take a new architectural functions such as 2-way SIMD, 256 floating point registers, etc… into account.

3.3 Programming Environment for Post-K Computer

We interviewed some scientists involved in developing applications for the post-K computer, to clarify challenges and problems on the programming environment of the post-K computer. The results are being investigated to make the basic design of the programming environment, such as languages, compilers, and tools. In addition, we made a plan of collaboration with the partner company in developing a compiler of XcalableMP PGAS language for the post-K computer.

4. Schedule and Future Plan

In 2015, we will continue to perform the basic design of the post-K computer and start detail design.
For the performance verification environment & tools, we will extend our simulator and compiler to FX100, which is a successor of K-computer and FX10, and extend it to the post-K computer. Also, we are developing a tool to obtain all the communication messages of an application through a parallel execution. These messages will be substituted into corresponding communication buffers when we analyze single node performance of the application on the simulator.
For the programming environment for the post-K computer, we will design and develop an XcalableMP compiler for the post-K computer, where important development items are supporting the latest standard of the base languages, cooperating with the backend compilers, leveraging a high-performance low-level communication layer, etc.

5. Publicaiton, Presentation and Deliverables

(1) Journal Papers

(2) Conference Papers

(3) Invited Talks

1. Mitsuhisa Sato, HPC research and development in Japan - Post T2K and post K project -,

EuroMPI/Aisa 2014.

2. Mitsuhisa Sato, Issues for Exascale Accelerated Computing - system architecture and programming, Exascale Applications and Software Conference 2014 - EASC2014.

(4) Posters and presentations

(5) Patents and Deliverables

(6) Awards

Application Development Team

1. Team members

Hirofumi Tomita (Team Leader)
Seiya Nishizawa (Research Scientist)
Kazunori Mikami (Research & Development Scientist)
Soichiro Suzuki (Research & Development Scientist)
Mamiko Hata (Technical Staff I)
Yukihiro Komura (Postdoctoral Researcher)
Naoya Maruyama (Research Scientist)
Jaewoon Jung (Research Scientist)
Yoshifumi Nakamura (Research Scientist)
Hisashi Yashiro (Research Scientist)
Chigusa Kobayashi (Research Scientist)
Yukio Kawashima (Research Scientist)
Shinichiro Takizawa (Research Scientist)
Motohiko Matsuda (Research Scientist)
Yosuke Murase (Research Scientist)
Michio Katouda (Postdoctoral Researcher)
Keiji Onishi (Postdoctoral Researcher)
Koji Terasaki (Postdoctoral Researcher)
Yuichi Otsuka (Research Scientist)
Toshiyuki Imamura (Research Scientist)

2. Research Activities

2.1. Co-design based on target applications

We execute the performance analysis and optimization of the “target applications” selected from nine social and scientific priority issues chosen by the advisory panel of MEXT.

Each of the target applications has its own scientific algorithm and scheme, each representing different computational workload characteristics such as floating point operations, successive and/or random memory operations, data transactions over network, external storage I/O, and more on.

Achieving the expected performance on post-K computer requires the in-depth study and optimized implementation effort by the application and the system design in collaborative manner.

This effort is integrated as the co-design of post-K computer.

The preliminary analysis of the target applications group 1 has been conducted for the basic design of the proposed system. The obtained information is being composed and will be reported to flagship 2020 project committee.

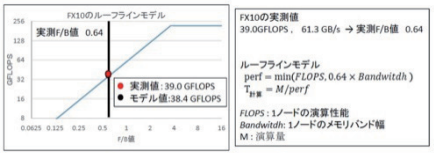
2.2. Development of an application benchmark suite for system performance evaluation

We develop and maintain the "mini-apps" that are designed to represent the same performance characteristics as full applications from major computational science domains. The mini-apps are small in program size, packaged for easy build and run, and are available in source code format, which is often not the case with the full applications. The mini-apps benchmark suite is the collection of such mini-apps, and is made available for public access in the Web page below:
http://fiber-miniapp.github.io/

We conducted the performance evaluation of ccs-qcd, ffvc_mini, marble_mini and ngsa-mini mini-apps in 2014. We built the performance models of those mini-apps and conducted the comparative study of the models and the actual measured performances.

Name	Calculation method	Parallelization method			Communication type
		MPI	OpenMP	OpenACC	
CCS QCD	Lattice QCS	✓	✓	✓**	Boundary + Collective
MARBLE	MD(PME)	✓	✓		Boundary + AlltoAll
MODYLAS	MD(FMM)	✓	✓		Boundary + Collective
FFVC	CFD	✓	✓		Boundary + Collective
NGS Analyzer	Genome Sequence Matching	✓			through the File I/O
NICAM-DC	Climate Simulations	✓	✓	ongoing	Boundary + Collective
mVMC	Quantum Monte Carlo	✓	✓		Collective

* as of Nov. 2014 ** external collaborator by Nvidia



2.3. Supporting activities to promote the community of computational science on Future HPC Infrastructures

We organized a working group for promoting computational sciences using future HPCI as continuing work of "Feasibility Study on Future HPC Infrastructures (Application Working Group)". The working group consists of researchers working on the frontline of various scientific communities and they discussed and confirmed the following issues;

- Continuing update of the "Science Roadmap" and cooperation with HPCI Consortium
- Promoting a common meeting ground of various fields of computational sciences

3. Publication, Presentation and Deliverables

(1) Conference Papers

小村幸浩、鈴木惣一朗、三上和徳、滝澤真一朗、松田元彦、丸山直也，「Fiber ミニアプリの性能評価」, SWoPP 2014 IPSJ SIG Technical Report:

(2) Posters and presentations

Yukihiro Komura, Soichiro Suzuki, Kazunori Mikami, Motohiko Matsuda, Shinichiro Takizawa, and Naoya Maruyama, “Fiber Mini Applications”, SC14 booth poster session

(3) Deliverables

Fiber mini-apps benchmark suite, http://fiber-miniapp.github.io/

Co-design Team

1. Team members

Junichiro Makino (Team Leader)
Keigo Nitadori (Research Scientist)
Yutaka Maruyama (Research Scientist)
Masaki Iwasawa (Postdoctoral Researcher)
Ataru Tanikawa (Postdoctoral Researcher)
Takayuki Muranushi (Postdoctoral Researcher)
Natsuki Hosono (Postdoctoral Researcher)
Miyuki Tsubouchi (Technical Staff)

2. Team Mission

The mission of the Co-design team is to organize the "co-design" between the hardware and software of the exascale system. It is unpractical to design the many-core complex processor of today without taking into account the requirement of applications. At the same time, it is also unrealistic to develop applications without taking into account the characteristics of the processors on which it will run.
The term "Co-design" means we will modify both hardware and software to resolve bottlenecks and achieve best performance.

In the early phase, the team lead the effort to estimate the performance of key applications on the new machine, find out the bottlenecks in both the hardware and software sides, and propose improvements.

In the late phase, the team will study the interaction between the hardware, system software, and applications, and investigate how the performance can be improved.

In addition, the team takes into account the direction of the evolution of processors, study the new algorithms which can better utilized the new hardware, and develop DSL (domain-specific language) and frameworks for application development, which help the implementation of new algorithms.

3. Research Activities

Significant part of the activities of Co-design team is related to the development of the exascale system, and cannot be made open here. We summarize some of the achievements of general interest.

a) Research related to high-performance DSL for stencil computations.
Stencil computations are generally believed to be bandwidth-limited, since the number of floating-point operations per grid point is not so large. However, recently, the idea of "temporal blocking" has become a hot topic. With temporal blocking, computation of multiple timesteps is applied to local subset of the computational domain, so that the bandwidth requirements is reduced. We developed a new algorithm for temporal blocking which can be parallelized over multiple cores and over multiple nodes of distributed-memory parallel machines without any increase in the number of floating point operations. In addition, we derived the relation between the maximum possible reduction in the bandwidth and the cache size. For problems in D-dimensional space, the maximum reduction is proportional to the cache size to the power of 1/D.

b) Research on ultra-many-core architectures and applications for them.
The direction of the advance of the semiconductor technology in the last decade, and also in the next decade, is that the available number of transistors increases while their speed remain constant. Thus, it has become very important to utilize a large number of cores to solve problems of relatively small size, since that is the only way to reduce the turnaround time of one simulation. As one example, we have studied the algorithm and network characteristics necessary to use very large number of cores for small-scale molecular-dynamics simulations.

It turned out to be possible to use one core to calculate one cell-cell interaction, or even to use multiple cores to calculate single cell-cell interaction, if on-chip and inter-chip networks have certain characteristics. The requirement for the communication bandwidth is not so high, such as around 100GB/s in total for a chip with peak speed of 20Tflops. The most important feature, which is not available on present-day many-core processors, is a reasonably efficient way to take reduction operations over group of cores which share the calculations related to one cell, and fast synchronization of cores to make use of such reduction.

4. Publications

(1) Journal Papers

(2) Conference Papers

1. “Nanoblock Unroll: Towards the Automatic Generation of Stencil Codes with the Optimal Performance”, Takayuki Muranushi; Keigo Nitadori, Junichiro Makino, Proceedings of the Second Workshop on Optimizing Stencil Computations, 49-55

(3) Invited Talks

1. 牧野淳一郎 エクサスケールマシン開発プロジェクトアクセラレーション研究会 @OIST2014/06/19-20

(4) Posters and presentations

(5) Patents and Deliverables

(6) Awards

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