Annual Report
2012-13

AICS Research Activities

July 2013

Contents

i Preface

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Director, Research Division

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It is our pleasure to report AICS's activities of research, development and operation of the K supercomputer during the period of April 2012 to March 2013. More than two years have passed since the research division of AICS was launched. Also, the operations and computer technologies division was newly formed in July 2012. The research division has been steadily growing. We have now 16 research teams and 3 research units. It has reached nearly its full scale that was originally expected in terms of the number of teams and units. Some research teams and units are relatively new and they are not in a complete form yet.

Making the world class supercomputer to work at its full potential requires extremely sophisticated technology. Achieving this kind of technology is impossible without close collaboration between computational science and computer science, and such collaboration is precisely what is taking place in AICS. This report in part tries to present the collaboration.

Of course, one of the most important missions of AICS is, to operate the K supercomputer effectively and efficiently for serving users from a wide variety of research areas. This mission has been carried out successfully by AICS's operation and computer technologies division. The division is not fully separated from the research division. The activities of the operation division include to make (and help making) application programs more parallelized and optimized. The performance, scheduling and recovering operations of the K supercomputer have been fully in control of the operation division. Its activities, which are vital to AICS, are reported as well.

ii Mission and Overview

Japan's Third Science and Technology Basic Plan (a Cabinet resolution adopted in March 2006) designated next-generation supercomputing as a key technology of national importance that should be the focus of investments in gestation periods for large-scale national projects. As a result, RIKEN along with the Ministry of Education, Culture, Sports, Science and Technology (MEXT) are putting full efforts into the development and advancement of such technology.

Under the guidance of MEXT and on the basis of the "Law on Joint Use Promotion of Large-Scale Advanced Research Facilities" (effective July 2006), RIKEN has been managing the construction of the Next-Generation Supercomputer, the "K computer." The K computer is to be a shared resource based on the above law and, with its wide accessibility, is expected to be put to a broad range of uses—from diverse fields of basic science and technology research to applications in industry. It was with this in mind that RIKEN established the Advanced Institute for Computational Science (AICS) on July 1, 2010. Through the use of its world-class supercomputer boasting 10 petaflops of computational power, and through collaboration and integration of the fields of computational science and computer science, AICS strives to create an international center of excellence dedicated to generating world-leading results. AICS's missions are:

1. Operating the K computer efficiently for users of wide research areas as well as of industries,

2. Carrying out the leading edge research of computational science and technology, and establishing itself as the COE of computational sciences in Japan.

3. Proposing the future directions of HPC in Japan.

And also, AICS's missions include:

- Promoting strong collaborations (or co-development) between computational and computer scientists, working with the core-organizations of the strategic areas identified by the Strategic Programs for Innovative Research (SPIRE),

- Raising and promoting young scientists who are strong in both computational and computer sciences, and

- Pursuing new concepts for the future HPC beyond the petascale (including exascale).

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

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

technology.

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

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

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

iii Organization

The organization of AICS (as of October 2012) is schematically shown below. The research teams in computer science and computational sciences are closely integrated into the Research Division. Operations of the K computer and researches on its advanced utilization technologies are conducted in the Operations and Computer Technologies Division.

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Director, AICS
├── Deputy Director, AICS
│   Senior Advisor
│   Associate Director, AICS
├── AICS Policy Planning Division
│   ├── AICS Strategic Planning Section
│   └── AICS Collaborations Section
├── AICS Research Support Division
│   ├── AICS General Affairs Section
│   ├── AICS Finance Section
│   └── AICS User Service Section
├── AICS Office for Research Communication
├── AICS Safety Center
├── Operations and Computer Technologies Division
│   ├── Facility Operations and Development Team
│   ├── System Operations and Development Team
│   ├── Software Development Team
│   └── HPCI System Development Team
└── Research Division
    ├── System Software Research Team
    ├── Programming Environment Research Team
    ├── Processor Research Team
    ├── Large-scale Parallel Numerical Computing Technology Research Team
    ├── HPC Usability Research Team
    ├── Field Theory Research Team
    ├── Discrete Event Simulation Research Team
    ├── Computational Molecular Science Research Team
    ├── Computational Materials Science Research Team
    ├── Computational Biophysics Research Team
    ├── Particle Simulator Research Team
    ├── Computational Climate Science Research Team
    ├── Complex Phenomena Unified Simulation Research Team
    ├── HPC Programming Framework Research Team
    ├── Advanced Visualization Research Team
    ├── Data Assimilation Research Team
    ├── Computational Chemistry Research Unit
    ├── Computational Disaster Mitigation and Reduction Research Unit
    └── Computational Structural Biology Research Unit
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1. System Software Research Team

1.1. Team members

Yutaka Ishikawa (Team Leader)

Atsushi Hori (Senior Scientist)

Keiji Yamamoto (Postdoctoral Researcher)

Balazs Gerofi (Postdoctoral Researcher)

Akio Shimada (Research Associate)

Yoshiyuki Ohno (Research Associate)

Masayuki Hatanaka (Research Associate)

Toyohisa Kameyama (Technical Staff)

1.2. 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 exa-scale computing.   There are several issues in carrying out future computing. Two research categories are taken into account: i) scalable high performance libraries/middleware, such as file I/O and low-latency communication, and ii) a scalable cache-aware, power-aware, and fault-aware operating system for next-generation supercomputers based on many core architectures.

Parallel file I/O is one of the scalability issues in modern supercomputers. One of the reasons is due to heavy metadata accesses. If all processes create and write different files, the metadata server receives so many requests by all processes not only at the creation time but also at writing data to each file. Two approaches have been conducted to mitigate this issue. One approach is to introduce a file composition technique that gathers multiple data generated by an application and stores these data into one or a few files in order to reduce the number of files accessed by processes. The other approach is to provide multiple metadata server in which the requests for metadata are sent to a metadata server resolved using hash function.

Increasing number of cores and nodes enforces strong scaling on parallel applications. Because the ratio of communication time against local computation time increases, a facility of low-latency and true overlapping communication and computation communication is desired. A communication library, integrated to the MPI library implementation in K computer, has been designed and implemented, that utilizes DMA engines of K computer. Each compute node of K computer has four DMA engines to transfer data to other nodes. If a communication library knows communication patterns in advance, it may utilize the DMA engines. Indeed, the feature of MPI persistent communication, standardized in MPI-1.0, allows the runtime library to utilize the DMA engines for data transfers involved in the persistent communication with restricted usage.

The system software stack developed by our team is designed not only for special dedicated supercomputers, but also for commodity-based cluster systems used in research laboratories. The system will be expected to be used as a research vehicle for developing an exa-scale supercomputer system. This is partially supported by JST CREST Post-Petascale research project.

1.3. Research Results and Achievements

1.3.1. Big data processing on the K computer

This research is conducted by collaboration between the Data Acquisition team of RIKEN Spring-8 Center and the System Software Research team of RIKEN AICS. The goal of this project is to establish the path to discover the 3D structure of a molecule from a number of XFEL (X-ray Free Electron Laser) snapshots. The K computer is used to analyze the huge data transmitted from RIKEN Harima where SACLA XFEL facility is located. Figure 1 and Figure 2 show an outline indicating how a molecule 3D structure can be obtained from images obtained by XFEL. Each image size is around 20 Mbytes, but may vary depending on the resolution of image sensor. However, the number of images required to develop a 3D structure of a molecule is millions, resulting 20 PBytes of data size in total. Further, each image is classified into thousands of images to have every possible snapshot orientations and to reduce the quantum noise.
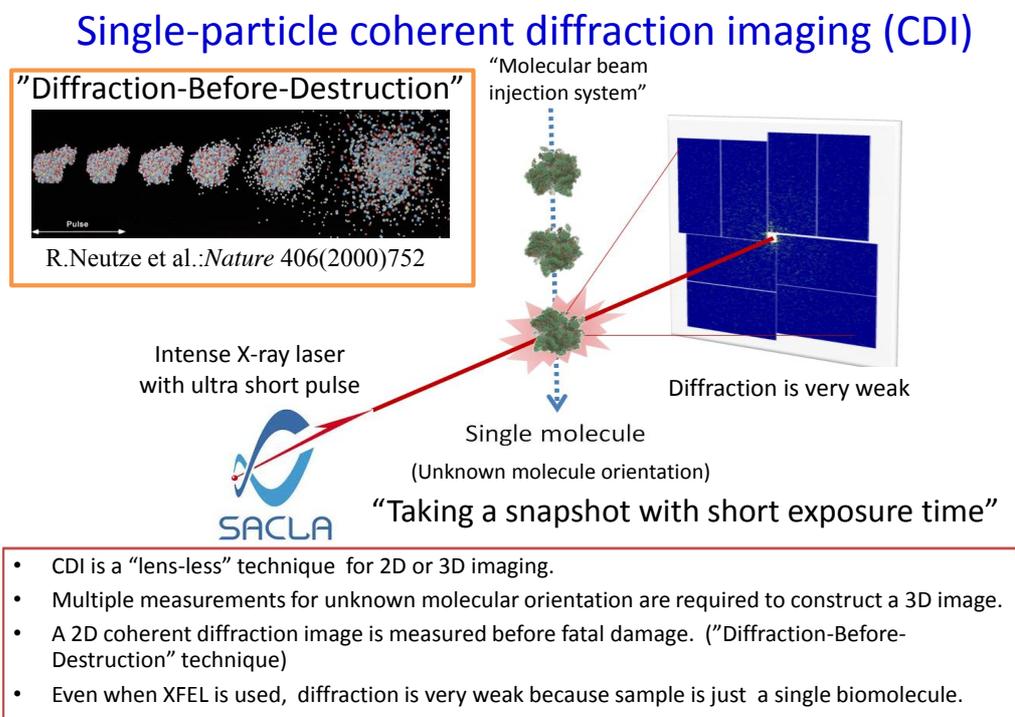
Figure 1 How SACLA XFEL works
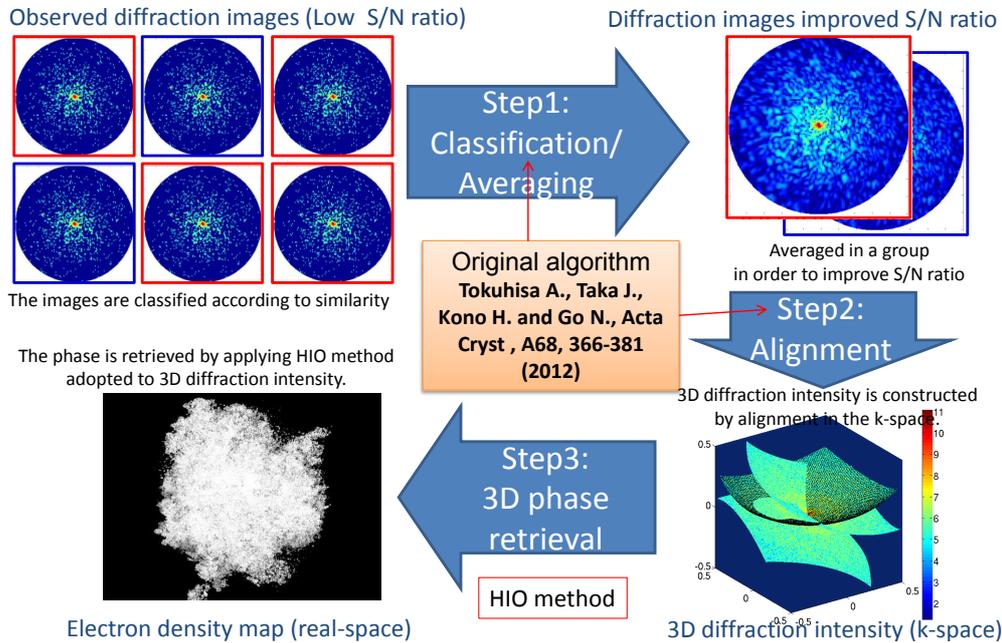
Figure 2 Obtaining electron density map from XFEL snapshots

The developed software consists of two parts. One is to select representative images and another is to classify images using selected representative images as shown in Figure 3. The classification is conducted by several FFT operations on each image to have correlation. The order of the number of this FFT operation to select thousands classification images is $O(M^2)$, followed by the classification of the rest of the images of $O(N*M)$ FFT operations, where M is the number of classification and N is the number of images. SACLA XFEL is going to produce 30 images in a second and the time to take one million images takes approximately 9 hours. There can be the cases where the snapshots are not well enough quality to analyze. In this case, the experiment must be stopped and tuned to obtain good quality images. Thus the image analysis must be done as soon as possible. This heavy computation, one million images should be analyzed as soon as possible, requires the power of the K computer. The Data Acquisition team at SCALA has been developing a classification algorithm, while the System Software Research team at AICS has been in charge of parallelization, performance tuning, and I/O. Since this is the first year of this project, the development of the software is the target. Performance tuning and I/O tuning are left in the following years.
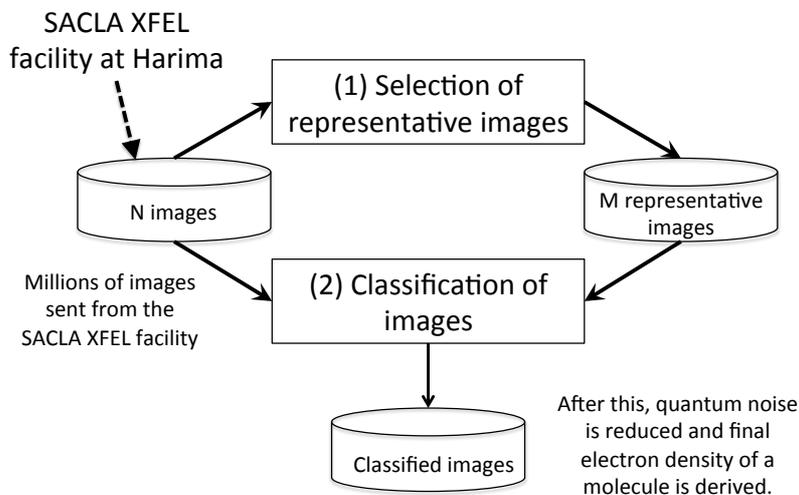
Figure 3 Block diagram of the procedure running on the K computer

1.3.2. File Composition Library

From FY2011, we have been developing a file I/O middleware called File Composition Library (FClib). FClib aggregates files created by parallel processes and stored to one of a few files. This results in reducing bottleneck of metadata operations on the metadata server.

In FY2012, FClib has been ported on the K computer based on the FY2011's implementation of commodity-based PC cluster. We measured the performance of FClib in case that each process creates/writes to one file into an aggregate file on shared directory. In order to compare with the regular file system provided by K computer, we measured the performance that each process creates/writes to one file to each rank directory. As shown in Figure 4, FClib performs 2.5 times faster than the original file I/O in the create operation, but 15-20 % of write throughput is dropped.

So various write access patterns have been measured to find out the source of performance degradation. It has been shown that if each compute node writes data to its associated directory, called rank directory, the write throughput is better than the case that writing data to a regular directory. This is because rank directories are provided by different file servers, and thus storage accesses are well distributed. We modified FClib so that each compute node accesses its rank directory. As a result, the write throughput of FClib is the same performance where each compute node accesses its rank directory (Figure 5).
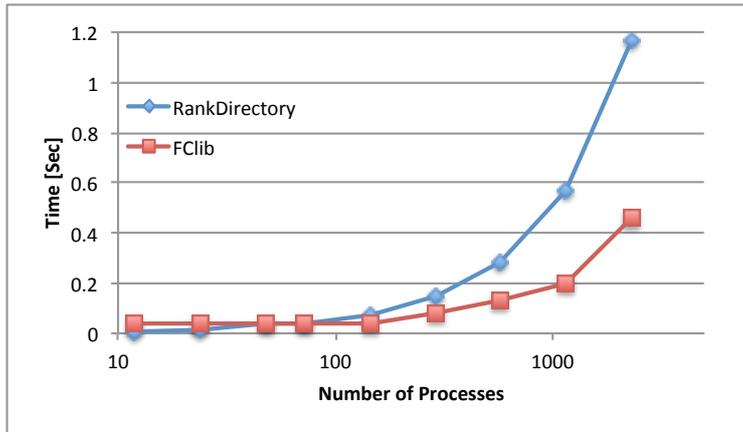
Figure 4 Elapsed time of file create
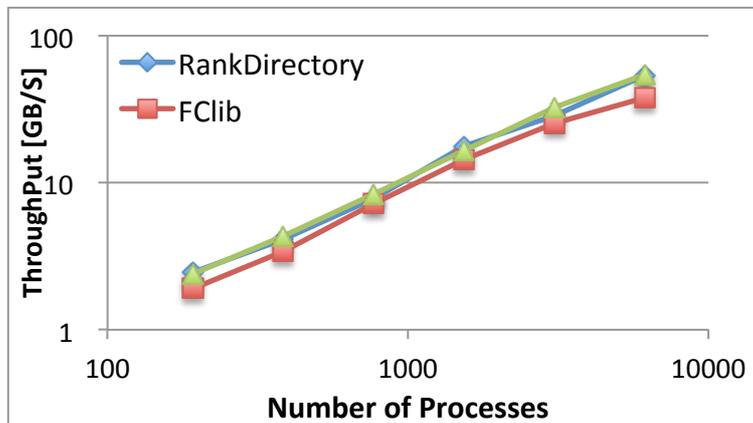
Figure 5 Write throughput of FClib

1.3.3. Hash-based Parallel File System

A parallel file system used in a modern supercomputer is basically composed of MDS (Metadata Server) and OSS (Object Storage Server). An MDS handles the file open, create and status operations. An OSS handles file read and write operations. Most current parallel file systems have only one MDS, and thus, such a system causes bottleneck of metadata operations requested by all compute nodes. A new scalable parallel file system based on a hash function has been designed and implemented from FY2011.

This system consists of multiple MDSs and OSSs as shown in Figure 6. Each MDS is responsible for metadata operations on a part of all files. The metadata set of files is determined by a hash value of the file name with path. The client determines the MDS of a file accessed in the client by a hash value of that file and path, and metadata operations for that file are sent to the MDS. The MDS informs the client to the location of OSSs for write/read operations in the client.
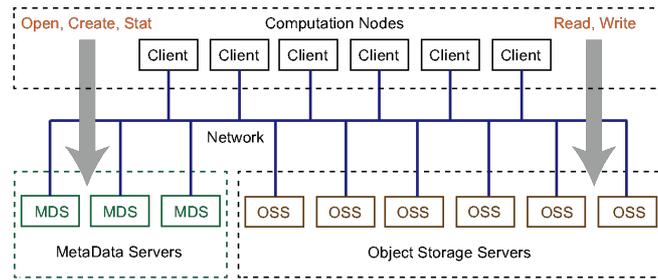
Figure 6 Hash-based Parallel File System

In FY2012, we implemented transactional metadata operations using software transactional memory for consistency of metadata. Two or more same operations are consistently executed at the same time. Evaluations show that file creation throughput of proposed file system is about 25 times higher than that of current Lustre File System in the case of 64 metadata servers as shown in Figure 7.
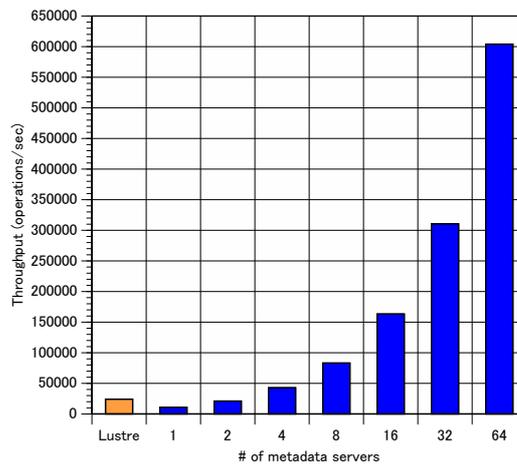
Figure 7 Throughput of the file creation

1.3.4. Persistent RDMA

The implementation of persistent communication provided in MPI has been reconsidered to provide low latency and true overlapping communication and computation. If the communication code is implemented using the persistent communication facility in the way that the end-points of both the sender and the receiver are set up by issuing MPI_Send_init and MPI_Send_recv primitives prior to actual communication triggered by the MPI_Start or MPI_Startall primitive. The same communication pattern is reused without reissuing the initialization. Thus, at the start of actual communications in persistent communication, the runtime system already knows all the communication patterns, i.e., peers and message sizes if both sender and receiver have issued persistent communication primitives. Such situations have

15

a chance for the communication library to utilize four DMA engines equipped in K computer and carry out true overlapping communication and computation.

FY 2012, a novel method to schedule DMA engines for K computer was designed and integrated into PRDMA (Persistent Remote Direct Memory Access) designed and implemented in FY 2011.
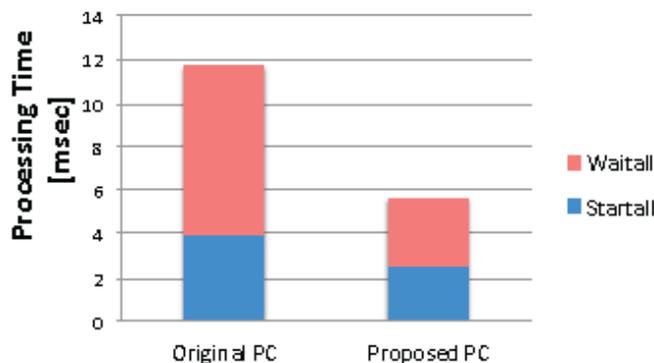
Figure 8 Comparison of original persistent communication and proposed one.

The proposed method was evaluated using a simple halo exchange program whose communication pattern is the same as a large eddy simulation code, SCALE-LES3. Figure 8 shows the evaluation results of using original and proposed persistent communication implementations. The proposed method is about two times faster than the original implementation.

1.3.5. New Process / Thread Model

We have been designing a new process / thread model that is suitable for the many-core architectures. The many-core architectures are gathering attention towards next generation supercomputers. Many-core architectures have a large number of low performance cores and the amount of the main memory per core is relatively small. On such environment, the system software should not consume a lot of memory.

The conventional process model has a problem in terms of the intra-node communication between parallel processes on many-core environments. It consumes a lot of memory in the kernel space for the intra-node communication using shared memory mapping scheme. In this scheme, shared memory regions are allocated on the memory, then each parallel process maps those shared memory regions to its own virtual address space. Parallel processes can communicate via those shared memory regions. However, a lot of page table entries are required to map the shared memory regions. For example, 200MB memory is consumed on the page table entries in the kernel space in case that parallel processes map the 1GB shared memory region to their own address space.

One of the solutions to solve this problem is to utilize a small shared memory region as just a intermediate buffer. In this method, parallel processes send and receive the data via the shared memory region allocated as an intermediate buffer. However, this method introduces two memory copies on the intra-node communication. These two memory copies can decrease the performance of the parallel application.

Partitioned Virtual Address Space (PVAS) is a new process model to achieve the low-cost intra-node communication on the many-core environments. In PVAS, multiple processes run in the same virtual address space as described in Figure 9 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 another process can be accessed by the normal load and store instructions, just like the same way accessing the data owned by itself. PVAS is designed not only to achieve high performance intra-node communication, but also to minimize the memory usage in the kernel space. PVAS processes do not have to map the shared memory regions for the intra-node communication because the address space boundaries between PVAS processes do not exist. Therefore, the page table entries to map the shared memory regions are not required.
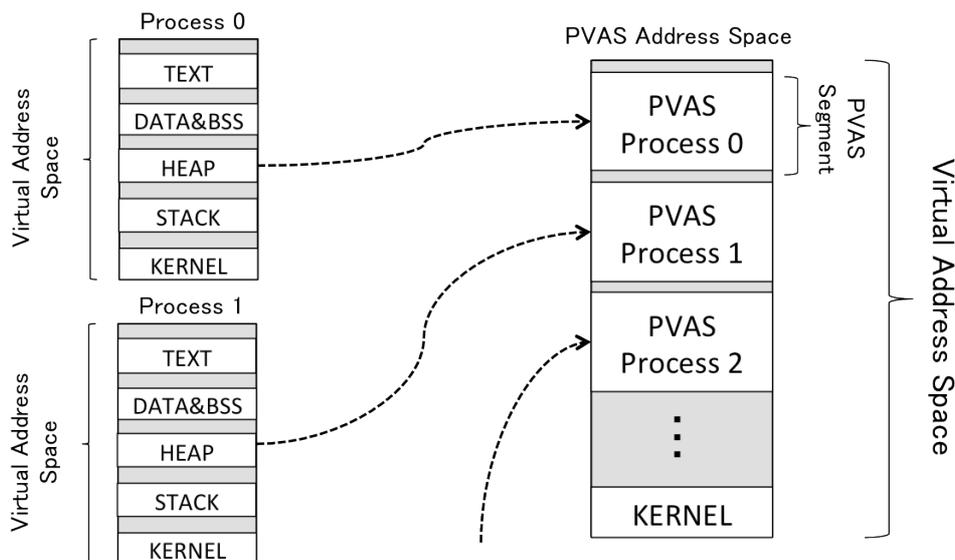
Figure 9 Semantics view of the Partitioned Virtual Address Space

We implemented the PVAS process model in the Linux kernel and modified the MPI communication library (MPICH2) to utilize the PVAS intra-node communication. Figure 10 shows the performance results of the ping-pong communication between a pair of processes utilizing MPI_Send() and MPI_Recv(). The latency of the PVAS implementation is faster than that of the Nemesis implementation that utilizes shared memory region as an intermediate buffer for the intra-node communication. Because the PVAS implementation introduces only one memory copy in the intra-node communication while the Nemesis implementation introduce two memory copies.
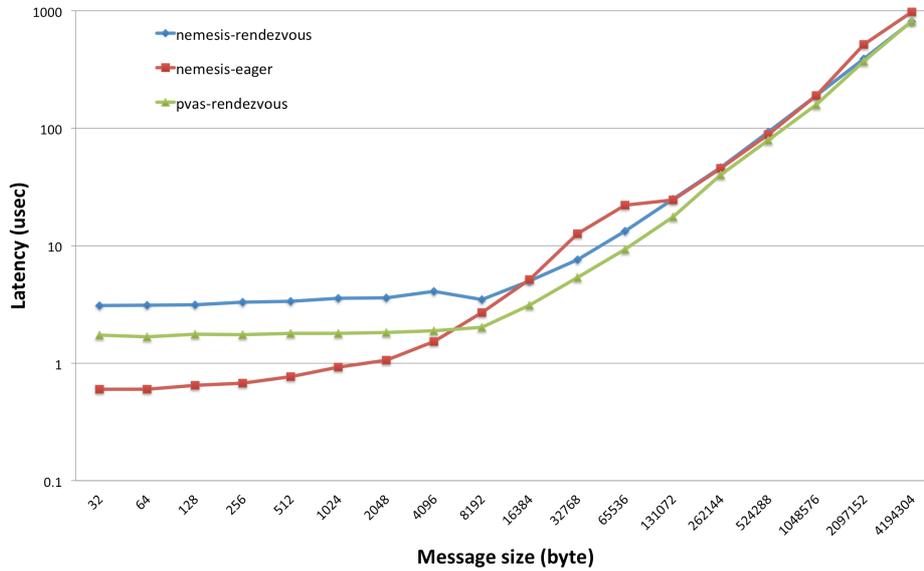
Figure 10 MPI ping-pong communication latency

We also evaluated the PVAS intra-node communication in PGAS language. We modified XacalableMP, which is one of the PGAS languages, to utilize the PVAS intra-node communication. XacalableMP implemented with the GASNet communication system for the intra-node communication. GASNet has two methods for the intra-node communication. First, GASNet-AM utilizes a shared memory region as just an inter-mediate buffer, and then two memory copies are required on the intra-node communication. In the other one, the GASNet-Shmem allocates a shared memory region as a global array and parallel processes map it to their own address space, therefore, only one memory copy is required on the intra-node communication.

Figure 11 shows the performance result of the NAS Parallel Benchmarks implemented by the XscalebleMP. A red bar represents the elapsed time for the intra-node communication and a green bar represents the elapsed time for the calculation.

The PVAS implementation is comparable with GASNet-Shmem, because it introduce only one memory copy as same as GASNet-Shmem. However, memory consumption of PVAS for the intra-node communication is fewer than that of GASNet-Shmem in theory.
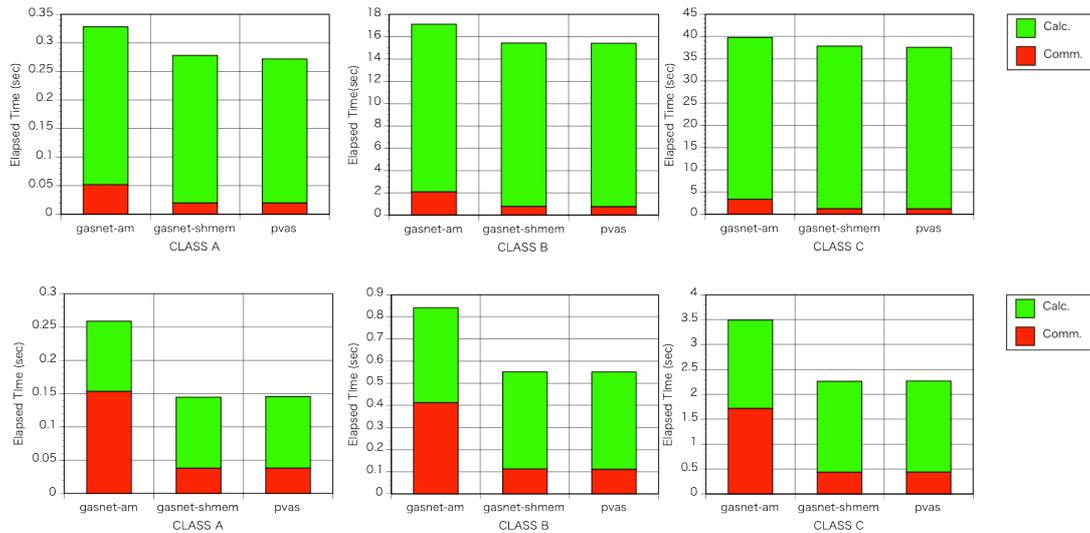
Figure 11 NAS Parallel Benchmarks

1.4. Schedule and Future Plan

PRDMA will be open to users in May of 2013. More optimization techniques will be developed to mitigate network contentions. FClib will be optimized for K computer, and will be open to users. File IO for SACLA XFEL will be redesigned based on the FY2012 research results. MPICH3, an MPI implementation for the MPI-3 standard, will be ported and enhanced in K computer.

The system software stack has been designed and implemented in cooperation with the University of Tokyo. In FY2013, PVAS and its related research topics will be much focused, and the operating system kernel will be mainly developed at the University of Tokyo.

1.5. Publication, Presentation and Deliverables

(1) Journal Papers

- None

(2) Conference Papers

1. PGAS Intra-node Communication towards Many-Core Architecture (Akio Shimada, Balazs Gerofi, Atsushi Hori, Yutaka Ishikawa), In 6th Conference on Partitioned Global Address Space Programing Model, 2012.

2. Yoshiyuki Ohno, Atsushi Hori, Yutaka Ishikawa, "File Composition Technique to Improve the Performance of Accessing a Number of Small Files", In Proceedings of the International Conference on Parallel and Distributed Processing Techniques and Applications, volume I, pages 395--400, 2012

(3) Invited Talks
   ‐ None

(4) Posters and presentations
   1.   Partitioned Virtual Address Space, In The 1st HPC in Asia Workshop, 2012.
   2.   Yoshiyuki Ohno, Atsushi Hori, Yutaka Ishikawa, "File Composition Technique for Improving Access Performance of a Number of Small Files", 10th International Meeting on High-Performance Computing for Computational Science (VECPAR 2012), 2012.
   3.   Keiji Yamamoto, Atsushi Hori, Yutaka Ishikawa, "Distributed Metadata Management for Exascale Parallel File System", SC12 The International Conference for High Performance Computing, Networking, Storage, and Analysis, 2012

(5) Patents and Deliverables
   PRMDMA will be distributed in May 2013.

2. Programming Environment Research Team

2.1. Team members

Mitsuhisa Sato (Team Leader)

Hitoshi Murai (Research Scientist)

Tetsuya Abe (Postdoctoral Researcher)

Swann Perarnau (Visiting Researcher, JSPS Research Fellow)

Tomotake Nakamura (Research Associate)

Takenori Shimosaka (Research Associate)

Masahiro Yasugi (Visiting Researcher)

Tomio Kamada (Visiting Researcher)

Hitoshi Sakagami (Visiting Researcher)

Hiroaki Umeda (Visiting Researcher)

Miwako Tsuji (Visiting Researcher)

Horitz Helias (Visiting Researcher)

Susanne Kunkel (Visiting Researcher)

Masahiro Nakao (Visiting Researcher)

Tomoko Nakashima (Assistant (Concurrent))

2.2. Research Activities

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

In 2012FY, in order to archive these objectives above, we carried out the following researches:

1) We continued the development of XcalableMP(XMP) programming languages. XcalableMP is a directive-based language extension which allows users to develop parallel programs for distributed memory systems easily and to tune the performance by having minimal and simple notations. The specification has been designed by XcalableMP Specification Working Group (XMP Spec WG) which consists of members from academia and research labs to industries in Japan. We have been working with XMP Spec WG to improve the specification. In this year, we released XMP Fortran, and deployed it to the K computer. According to the results from a preliminary performance evaluation using a XMP version of the SCALEp code (a climate code for LES), we improved the runtime system on the K computer. We conducted the evaluation of

XMP programs on the K computer using HPCC benchmark and submitted the results to SC12 HPCC class 2 competition, and were selected as a finalist. We also continued the design of the interface to MPI programs in XMP, and IO supports of the XMP language.

2) For the research for performance tuning tools for large-scale scientific applications running on the K computer, we have ported the Scalasca performance turning and analysis tool developed by JSC, Germany, to the K computer. Our update on the Scalasca for the K computer was included in the formal release.

3) We investigated methods and tools to support a correct parallel program. We proposed a light-weight XMP verification tool which helps users to verify XMP programs using descriptions of global-view programming directives in XMP. And also, we studied the model checking technique of the PGAS language including XMP.

4) The processor of the K computer has an interesting hardware mechanism called "sector cache", which allows partition of L2 on-chip cache to optimize the locality for important data. We published a paper about the technique to optimize the usage of sector cache.

5) We joined Japan-France project FP3C, "Framework and Programming for Post Petascale Computing", from this year. In this year, we worked on porting and performance evaluation of the integrated programming environment of XcalableMP and YML which is developed by the French team.

6) We conducted several collaborations on the performance evaluation with JSC, University of Tsukuba and other groups.

2.3. Research Results and Achievements

2.3.1. Development of XcalableMP and Performance Evaluation on the K computer

We continued the development of XcalableMP compiler in collaboration with University of Tsukuba. At the last SC12, the version 0.6 which includes the implementation of XMP Fortran as well as XMP C has been released. Several members of our team joined the XMP specification Working Group to update the XMP language specification to version 1.1 which was published at SC12.

Several performance evaluation of XcalableMP programs were conducted on the K computer. One of the important results was that of HPC Challenge Benchmarks. We have submitted the results to the SC12 HPC Challenge Benchmark, Class2 Competition, which was selected as a finalist.

In the evaluation of HPCC Benchmarks, we presented our XcalableMP implementation of the HPCC HPL, RandomAccess, FFT, and the Himeno benchmark which is a typical stencil application.

We have measured the performance of HPCC benchmark on two systems: The K computer, upto 8129 nodes, and HA-PACS system at University of Tsukuba, upto 64 nodes. Table 1 shows the

specifications of two systems. Figure 1,2,3,4 shows the performance and scalability of each benchmark respectively.

	The K computer	HA-PACS
CPU	SPARC64 VIIIfx 2.0GHz 8Cores, **128GFlops**	Xeon E5-2670 2.6GHz x2 8Cores x2, **332.8GFlops**
Memory	DDR3 SDRAM **16GB** **64GB/s/Socket**	DDR3 SDRAM **128GB** **51.4GB/s/Socket**
Network	Torus fusion six-dimensional mesh/torus network, **5GB/s**	Infiniband QDRx2rails Fat-tree network, **4GB/s**

Table 1. Specification of K computer and HA-PACS
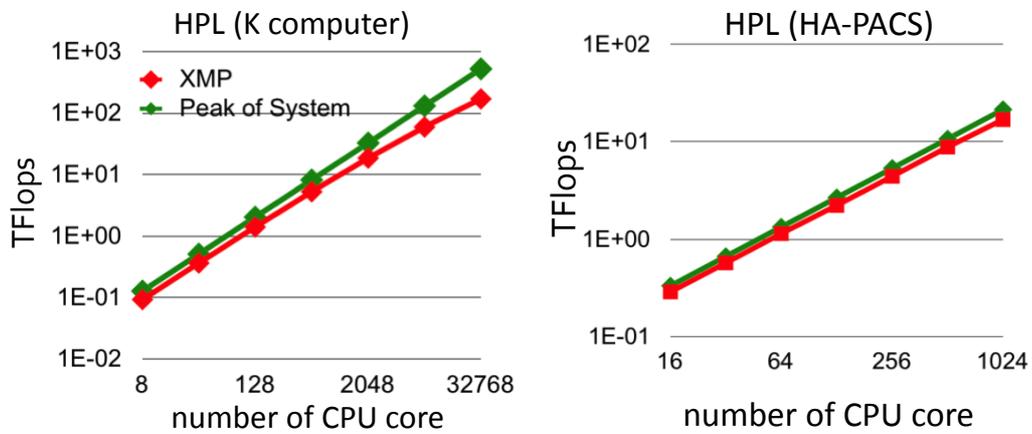
Fig 1. Performance and Scalability of HPL
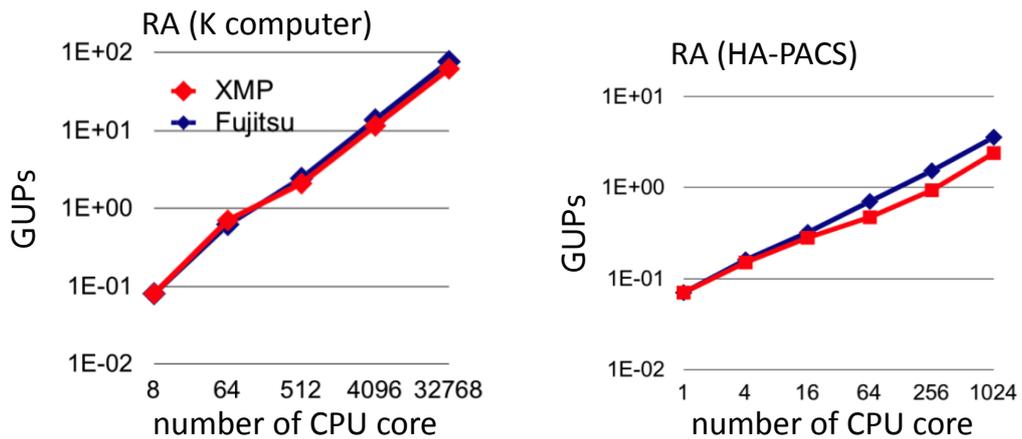
Fig.2　Performance and Scalability of Random Access
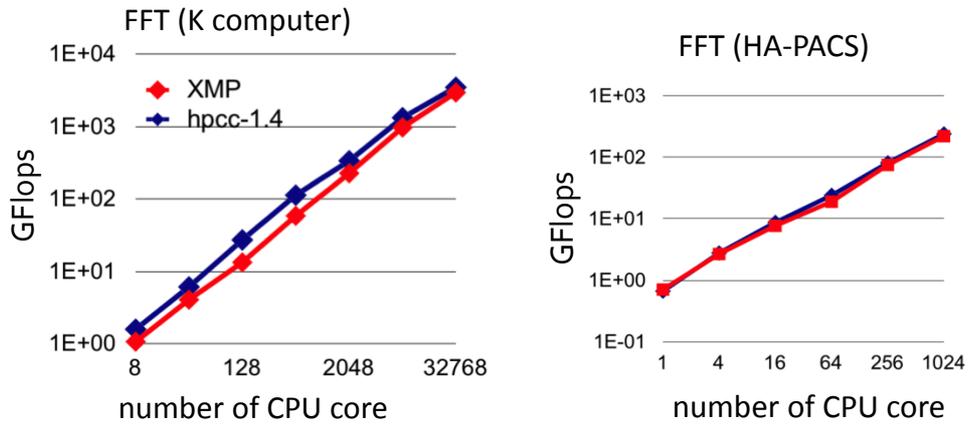
Fig. 3 Performance and Scalability of FFT
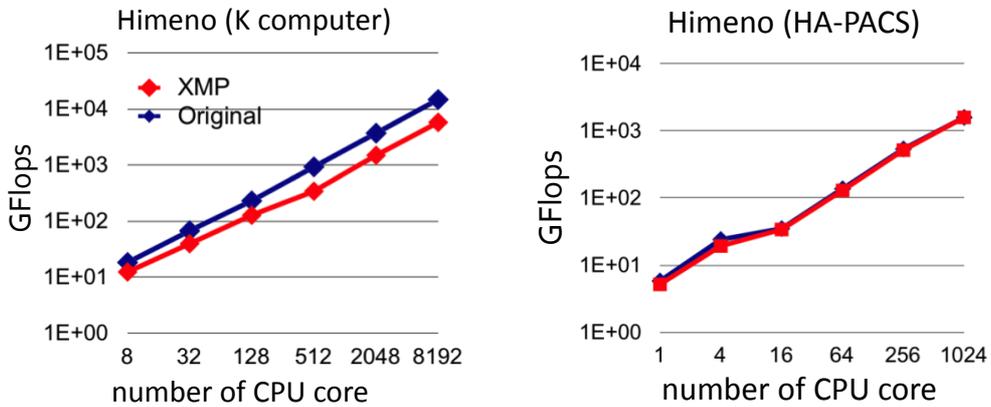
Fig.4 Performance and Scalability of Himeno

Overall, we found the performance gap between the XMP implementation and its counterpart in the K computer, while in HP-PACS the performance of the XMP implementation is very close to the original one. We already found and fixed some problems of the XMP in the run-time system and the algorithms.

Other important factor of programming languages is programability: how easy to program by the language. Figure 5 shows the source line of code (SLOC) of each benchmark programs in XMP comparing to the original MPI implementation as a reference. It means that the XMP can help the programmers to write programs with less lines, resulting in high programmability.
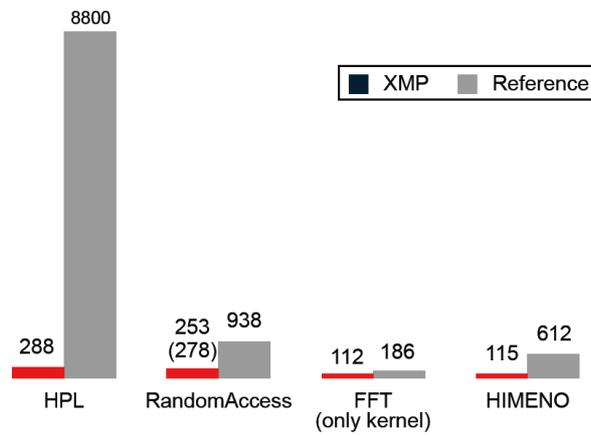
Fig. 5. Source Line of Code (SLOC)

2.3.2. Porting Scalasca performance tool to the K computer

We have ported Scalasca performance tools developed by Julich Supercomputer Center and German Research School for Simulation Sciences, and University of Tennessee, on the K computer. It is designed to analyze parallel application execution behavior on large-scale systems with many thousands of processors such as the K computer. It offers an incremental performance-analysis procedure that integrates runtime summaries with in-depth studies of concurrent behavior via event tracing, adopting a strategy of successively refined measurement configurations.

Our effort for porting the Scalasca to the K computer was included in the latest release 1.4.3. We have tested the tool to analyze the performance of CG in NAS Parallel benchmark using 16,384 nodes on the K computer. The view of the tool is shown in Figure 6.
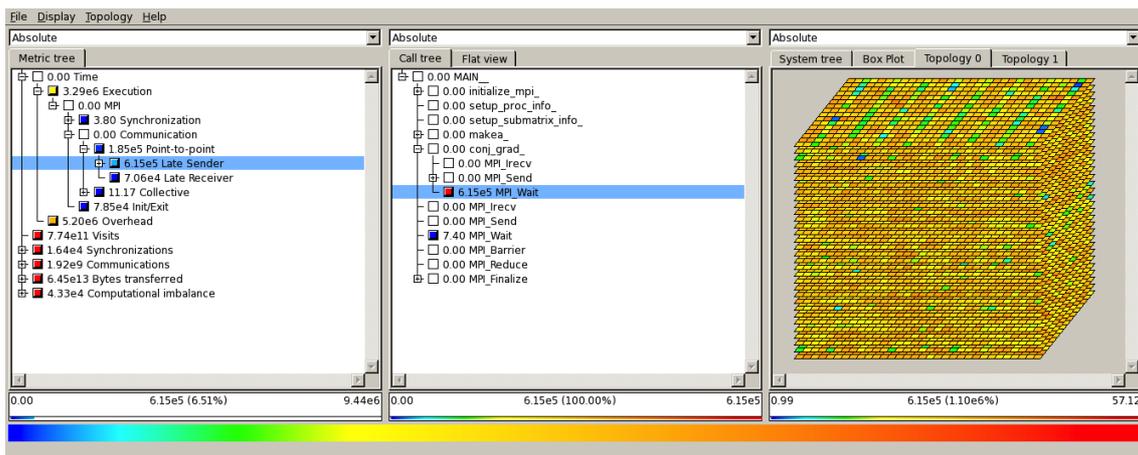
Fig. 6. View of Scalasca performance tool on K computer

(NPB CG benchmark, 32x32x16, 16,384 nodes)

2.3.3 Program Verification Techniques for PGAS programming models

In XcalableMP (XMP), programmers can include explicit synchronizations by adding directives to their source code. In this sense, XMP provides programmers with performance awareness. As such, part of the performance of programs can be attributed to the programmers, i.e., XMP requires interactive programming by the programmers.

We developed a tool that alerts programmers to missing and redundant synchronizations they have included referring, respectively, to non-local array indices and a decrease in the performance of programs. The tool uses XMP directives, making programs more structured, and on-the-fly checks whether directives are missing or redundant, while programmers are editing their programs.

Consider the code fragment shown below, the first pragma line specifies the broadcast operation of data a from node p(1) to nodes from p(2) to p(10), and the second pragma lines performs the broadcast the data from node p(2) to nodes from p(11) to p(20). Then, the third line which performs the broadcast from p(1) to p(10) and p(10), can be detected as a redundant operation. by our tool.

```
#pragma xmp bcast (a) from p(1) on p(2:10)
#pragma xmp bcast (a) from p(2) on p(11:20)
#pragma xmp bcast (a) from p(1) on p(10:11)
```

In the second example shown below, the array a is declared as a distributed array with block distribution. In the XMP execution, each node executes the same code independently if no xmp pragmas are specified. This means the assignment b=a[0] is executed on every nodes, and it causes the error on nodes where a[0] is not allocated. This kind of errors can be easily detected by static semantics check of our tool.

```
#pragma xmp distribute t(block) onto p
int i;
int a[100];
#pragma xmp align a[i] with t(i)
...
b=a[0];
```

We designed a light-weight static checking program for our tool, which is implemented by using a parser combinator library Parsec, and user-defined datatypes in Haskell performing pattern-matchings by constructors of the user-defined data types. And the tool is integrated with GNU Emacs editor. The pragma and the line containing passible errors are high-lighted in the editor, as shown in Figure 7.

Figure 7. Integrated environment with Emacs

Through the development of our tool, we found that abstract descriptions in XMP are useful to not only development of a program but also verification of the program.

One of the problems with PGAS languages including XcalableMP is that programmers can easily introduce concurrency bugs into their programs. For example, race conditions tend to occur because a portion of a single address space can be manipulated by multiple threads simultaneously. A solution that avoids race conditions is to synchronize accesses from multiple threads with synchronization primitives (e.g., synchronization locks), but this is not that easy for two reasons. First, excessive use of synchronization may severely degrade the performance of the program. Second, synchronization primitives themselves sometimes introduce other problems. For example, improper use of synchronization locks may cause deadlock.

Model checking is one approach for addressing the problem of concurrency bugs. Basically, software model checking explores all the states that can be reached by executing a given program, and checks whether a given property is ensured (e.g., there are no race conditions or deadlock).

Model checking of partitioned global address space programs tends to suffer from the state explosion problem because these programs allow concurrent and/or parallel execution and memory sharing. To avoid this problem, it is essential to perform proper abstractions based on the properties to be verified because these can dramatically reduce the number of states to be explored in programs. However, it is not always easy to automatically infer proper abstractions because programs and properties to be verified vary.

To address the problem, we proposed a model checking framework that includes user-definable

abstractions. The key idea of the framework is that it exposes the intermediate representation of the program's abstract syntax tree, enabling users to define their own abstractions flexibly and concisely by creating a translator for the tree. By allowing users to create translators at the level of abstract syntax trees, the cost of implementing the translator is lower than that of coding text-based pattern matching and rewriting rules because unnecessary redundant rules that often appear in the conventional approach are eliminated.

In addition, we have designed our proof-of-concept implementation of the proposed approach: CAF-SPIN. CAF-SPIN is a software model checking tool for Coarray Fortran (CAF) programs. In the current implementation of CAF-SPIN, both its intermediate representation of abstract syntax trees and translator are written in Haskell. Thus, users are able to define their abstractions by simply writing Haskell functions. Several experimental results using CAF-SPIN were conducted. The experimental results confirmed that abstractions can be defined easily and concisely in CAF-SPIN, and the number of states to be explored for model checking is dramatically reduced with the abstractions.

It is worth noting that, similar to UPC-SPIN, the current CAF-SPIN does not handle relaxed memory models directly, except for sequential consistency. This limitation does not cause problems for checking programs that perform synchronization when accessing shared memory, but may cause problems if synchronizations are accidentally or intentionally omitted for performance reasons. Supporting relaxed memory models is a future work.

2.3.4 "Sector Cache" optimization for the K computer

The processor architecture available on the K computer (SPARC64 VIIIfx) features a hardware cache partitioning mechanism called sector cache. This facility enables software to split the memory cache in two independent sectors: data loads in one sector cannot trigger the eviction of data in the second one. Moreover, software is responsible for data placement in each sector by issuing special instructions tagging the various memory loads performed during execution. The implementation details of this cache partitioning mechanism also enable fast redistribution of the cache during an application's runtime, without any cost, allowing any optimization using the sector cache to be applied multiple times, with different setups, in the event of phase changes.

Unfortunately, in its current state, the compilers provided on the K computer do not implement any automatic optimization using this cache facility. In the contrary, the only high-level interface to this mechanism is a set of directive to instruct the compiler to generate tagging instructions over a code region. Thus, only application programmers with intricate knowledge of both the memory access patterns of their code and the K computer architecture can take advantage of this facility.

To address this issue and to study new optimization schemes using cache partitioning, we investigated a framework using binary instrumentation and reuse distance analysis to discover the

locality of important data structures in an application and to suggest appropriate data distribution schemes for the sector cache. These optimizations are then translated into calls to the source-level API provided by the K computer compilers.

Our framework leverages and extends several existing methodologies. First, we use binary instrumentation of the target application along with debug information parsing to trace the various memory accesses to major data structures of a code region. This trace is then analyzed using a derivative of reuse distance to assess the locality of theses structures. Third, by modeling the impact of these localities on the performance of the application, we identify whether cache thrashing could be reduced by isolating some of these data structures to a specific sector. We envision these components as steps in an optimization loop: after identifying cache performance hotspots, a developer can analyze them, use the sector cache API to optimize them and repeat the process as much as required.

We applied our framework to analyze and optimize a set of HPC benchmarking applications and demonstrate significant performance improvements.

We analyzed two benchmarks from the Omni OpenMP C version 2.3 of the NAS Parallel Benchmarks: CG, LU, and applied our framework. These benchmarks were only using one thread. In both cases, significant optimizations were found.

Most of the computation time of the CG benchmark is spent inside the conj_grad function. This function does not call any other, and is repeated multiple times during the benchmark's lifetime. The core of this function is a sparse matrix-vector product, with most of the memory accesses touching 3 data structures: the sparse matrix a, the column index colidx and a dense vector p. We analyzed the locality of these structure and, unsurprisingly, our framework indicated that the p vector could benefit for isolation using the sector cache. Indeed, both other structures exhibit streaming access patterns due to indirect accesses that could impact negatively the caching of p. Our optimization thus isolates p in sector 1, with enough space to allow good caching. Such optimization, adding only two lines to the source code of the benchmark reduces the execution time of this function by 10%.

Our process to analyze and optimize the LU benchmark was as follows. First, LU spends almost all of its runtime in the ssor function. This function contains a loop, calling successively several subroutines over shared data structures. Iteratively, these calls solves a system of Navier-Stokes equations by successive over relaxation, decomposing it into lower and upper triangular matrices. Overall, eight structures are of interest here: flux, u, rsd and frct, which are global arrays used as input and results storage, and a,b,c and d which are working arrays used across subroutines to hold partial results (triangular matrices). To analyze this benchmark, we configured our framework to trace recursively all instructions of the ssor function or of any other function called from it. The resulting analysis identified each of a, b, c and d to benefit from the sector cache in the same way.

The cache requirements of the other arrays could not fit in any sector configuration. While isolating only one of the 4 arrays identified by our framework only improved by 2% the benchmark's execution time, another optimization gave more interesting results. Indeed, protecting those 4 arrays for streaming accesses to the other variables of the program by pushing them all together in sector one proved to be a better optimization. It resulted in a 8% reduction of execution time of this function. We should note that, as the ssor function passes these arrays to some subroutines as parameters, we had to change the sector cache directives in them to match the actual parameter names. Overall, code modification added 10 lines of directives: for each of the 5 functions, one line for sector size and one for variable isolation. We excluded two functions (rhs and l2norm) from these modifications, as they do not use these arrays.

Table 2 describes the exact optimization on each benchmark's functions, and the resulting improvements. Note that the cache misses reduction reported are direct cache misses: cache misses triggered by the speculative hardware prefetcher are ignored.

Benchmark	Function	Isolated Variables	Sector Size	Miss Reduction (%)	Runtime Reduction (%)
CG	conj_grad	p	(1,11)	19	10
LU	ssor	a,b,c,d	(2,10)	48	8
	blts	ldz,ldy,ldx,d		75	10
	buts	d,udx,udy,udz		18	3
	jacld	a,b,c,d		64	14
	jacu	a,b,c,d		57	6

Table 2.Results of Optimization of NAB benchmarks (GC and LU)

2.4. Schedule and Future Plan

At the end of 2012FY, we have released the XcalableMP C and Fortran, and Scalasca for the users of the K computer. The important goal is to organize collaborations with application developers and improve our software. As one of activities for this goal, we have a plan to organize hands-on meeting with them. Through these case studies, we will extend it for valuable performance analysis in the K computer.

As a research agenda especially for the K computer, we will focus on the design on one-sided communication using K computer's RDMA hardware. We expect that it will contribute the scalability of large-scale applications for the K computer.

2.5. Publication, Presentation and Deliverables
(1)   Journal Papers
- None

(2) Conference Papers

1. Masahiro Nakao, Hitoshi Murai Takenori Shimosaka Mitsuhisa Sato. "XcalableMP for Productivity and Performance in HPC Challenge Award Competition Class 2", SC12 The 2012 HPC Challenge Awards BoF, Salt Lake City, Utah, USA, Nov., 2012.

2. Tatsuya Abe, Toshiyuki Maeda, and Mitsuhisa Sato., "Model checking with user-definable abstraction for partitioned global address space languages.", In Proceedings of the 6th Conference on Partitioned Global Address Space Programming Models (PGAS), Online. Santa Barbara, October 2012.

3. Tatsuya Abe and Mitsuhisa Sato. On-the-fly synchronization checking for interactive programming in XcalableMP. In Proceedings of the 5th International Workshop on Parallel Programming Models and Systems Software for High-End Computing (P2S2), pages 29--37. Pittsburgh, September 2012.

4. Tatsuya Abe and Mitsuhisa Sato. "Auto-tuning of numerical programs by block multi-color ordering code generation and job-level parallel execution.", In Proceedings of the 7th International Workshop on Automatic Performance Tuning (iWAPT), volume 7851 of Lecture Notes in Computer Science. Springer, Kobe, July 2012.

5. Swann Perarnau and Mitsuhisa Sato, "Discovering Cache Partitioning Optimizations for the K Computer," in proceedings of APPLC'13 workshop, Shenzhen, 2013.

[not refereed, in Japanese]

1. Tomotake Nakamura and Mitsuhisa Sato, "Performance Analysis using the performance analysis tool Scalasca on the K computer", IPSJ SIG Technical Report (in Japanese), Vol. 2012-HPC-135, pp.1-7, 2012.

2. Hitoshi Murai, Takenori Shimosaka and Yoshiyuki Ohono, Hisashi Yashiro, Hirofumi Tomita and Mitsuhisa Sato, "Performance Evaluation of Parallel Programming Language XcalableMP on the K Computer", IPSJ SIG Technical Report (in Japanese), 2012-HPC-135(44), (2012).

3. Toward Automated Cache Partitioning for the K Computer, Swann Perarnau and Mitsuhisa Sato, IPSJ SIG Technical Report , Okinawa, 2012.

(3) Invited Talks

1. Mitsuhisa Sato, "The next step for Post-Petascale Computing in Japan", HPC in Asia Workshop, ISC 2011, June 2012.

2. Mitsuhisa Sato, "XcalableMP PGAS parallel programming language for productive high-performance scientific programming", International Top-level Forum on Engineering Science and Technology Development Strategy, 2012 International Forum on HPC Challenges in China, Oct 2012

3. Mitsuhisa Sato, "The K computer and XcalableMP parallel language project --- Towards programming environment for productive high-performance scientific programming ---", ComPAR 2013, Jan 2013

(4) Posters and presentations

1. Hitoshi Murai, Masahiro Nakao, Takenori Shimosaka, Mitsuhisa Sato. "Implementation and Evaluation of HPC Challenge Benchmarks with the Omni XcalableMP compiler", The 3rd AICS International Symposium, Kobe, Hyogo, Japan, Feb, 2013.

2. Tatsuya Abe and Mitsuhisa Sato. Auto-tuning of numerical programs by block multi-color ordering code generation and job-level parallel execution. Poster Session in HPC in Asia Workshop, Online. Hamburg, June 2012.

(5) Patents and Deliverables

1. XcalableMP compiler ver. 0.6 (C and Fortran95) for the K computer
2. Scalasca performance analysis tool for the K computer
3. Xcrypt for the K computer
4. GASnet one-sided communication Library for the K computer (test version)

3. Processor Research Team

3.1. Team members

Makoto Taiji (Team Leader)

Gentaro Morimoto (Research Scientist)

3.2. Research Activities

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

In future high performance computing, we have to tackle with millions or more parallel operation units to extend the performance. However, many applications require acceleration while keeping the problem size, i. e. the strong scaling, and they can often be parallelized up to thousands of core, not to millions. To achieve better strong scaling, we have to decrease the cost of parallelization by improving the latency in everywhere – network, main memory, and processors. For this, we will try to develop the platform of System-on-Chip (SoC) based accelerators. It consists of general-purpose processor cores, memories, network units and computing accelerators on the single chip. By such integration we aim to achieve the ultimate performance for selected applications.
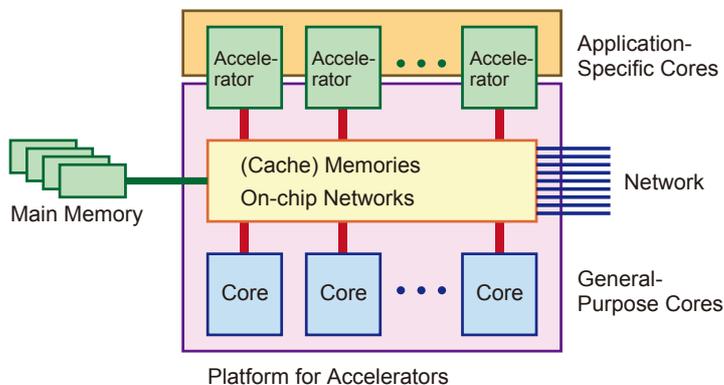
Fig. 1. Diagram of platform for accelerators.

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

3.3. Research Results and Achievements

3.3.1. Platform of accelerators

In this year we continued the design of the MDGRAPE-4 SoC in RIKEN QBiC (Quantitative Biology Center). 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.
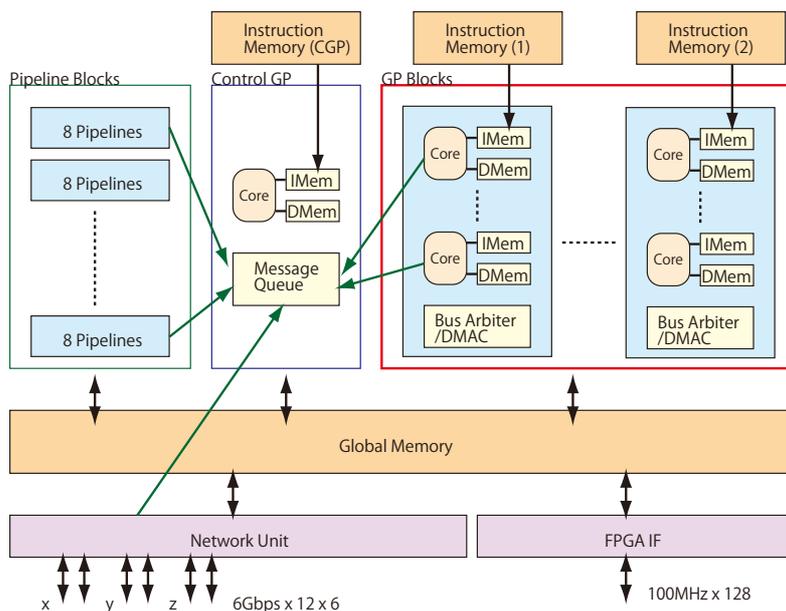
Fig. 2. Block diagram of MDGRAPE-4 SoC.
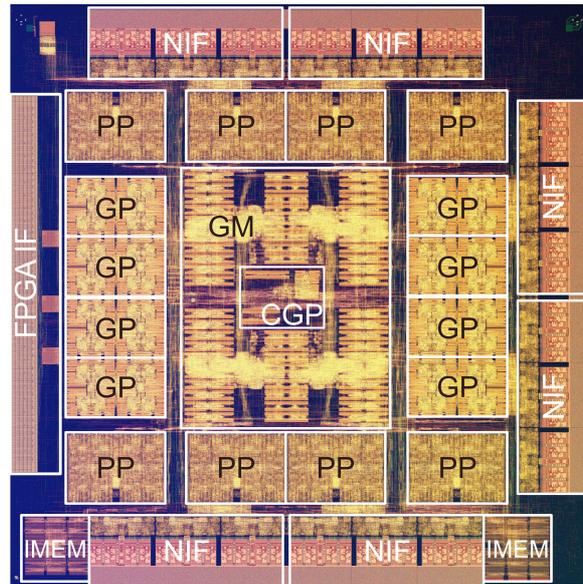
Fig. 3. Layout image of MDGRAPE-4 SoC.

3.3.2 Application Optimization on K computer

For application optimization we have optimized the molecular dynamics core code in collaboration with the Next-generation Integrated Simulation of Living Matter project.

3.4. Schedule and Future Plan

In the next year, we will finish the MDGRAPE-4 System in RIKEN QBiC. In future, we will continue to implement the part of the MDGRAPE-4 SoC as the platform of accelerators. We will also develop simulation environments for such system at RTL-level and behavior level. We will continue the optimization of MD core and the other codes for the K computer.

3.5. Publication, Presentation and Deliverables

(1)   Journal Papers

-None

(2)   Conference Papers

-None

(3)   Invited Talks

Makoto Taiji, "Accelerated Molecular Dynamics Simulations using Dedicated Hardware", International Supercomputing Conference 2012, Hamburg, 20 May 2012.

Makoto Taiji, "K-computer and its application to life sciences", BioIT CloudSummit, San Francisco, 11 September 2012.

Makoto Taiji, "INGENIOUS: Using next generation computers and algorithms for modeling the dynamics of large biomolecular systems", G8 Exascale Projects Workshop, Salt Lake City, USA, 12 November 2012.

Makoto Taiji, "MDGRAPE-4: a special-purpose computer for molecular dynamics simulations", UK-Japan workshop on High Performance Modeling of Multiscale Biomolecular Systems, 18 December 2012.

(4)   Posters and presentations
      -None

(5)   Patents and Deliverables
      -None

4. Large-scale Parallel Numerical Computing Technology Research Team

4.1. Team members

Toshiyuki Imamura (Team Leader)

Yoshio Okamoto (Visiting Researcher)

Yukiko Hayakawa (Assistant)

4.2. Research Activities

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

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

1) System of linear equations,

2) Eigenvalue problems,

3) Singular value decomposition,

4) Fast Fourier transforms, and

5) Nonlinear equations.

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

a) Tofu interconnect,

b) Parallel I/O,

c) Fault detection (soft-error), and

d) Higher accuracy computing.

We are going to complete this project through close collaboration among computational science (simulation), computer science (hardware and software) and numerical mathematics. Our final goal is to establish a fundamental technique to develop numerical software libraries for next generation supercomputer systems based on strong cooperation within AICS.

4.3. Research Results and Achievements

In this report, we mainly focus on three topics, 1) development of KMATHLIB, 2) collaborative work with JAEA, and 3) CREST project. Other activities done in FY2012-2013 can be referred from

the future plans and the publication list.

4.3.1. Development of KMATHLIB

Benchmarking OSS (Open Source Software) packages

We recognize that numerical library is an important tool to support simulation users when they develop their own practical codes on the K computer. Usage of the K computer is spread over a wide range of spectral from hundred to ten-thousand nodes or up to the whole system. Thus, to support such users widely is a very challenging work.

On the FY2012-2013, we researched and examined the availability of OSS (Open Source Software) packages, some of which have been ported to the K computer. To complete this work, we developed a benchmark suite at first. By using this benchmark suite and the standard profiling tool on the K computer, we measured several performance metrics, for example parallel efficiency, parallel speedup, and communication overhead. In order to utilize the computational potential of the K computer, we, especially, would like to know the parallel behavior defined by such as parallel efficiency, load balance and communication overhead. Figure 1 is an example of the benchmark suite. It illustrates the parallel performance of `pdgesv' and `pdhseqr' of ScaLAPACK on the K computer.

The benchmarking on this FY2012-2013 covers ScaLAPACK (pdgesv and pdhseqr), PETSc (GMRES and JD), and FFTW. We already run the benchmark code from 2^4=16 nodes (=128 cores) to 2^{15}=32768 nodes (=262144 cores). Currently, the benchmark is in the analyzing phase for the obtained results. Detail will be revealed in the FY2013-2014.
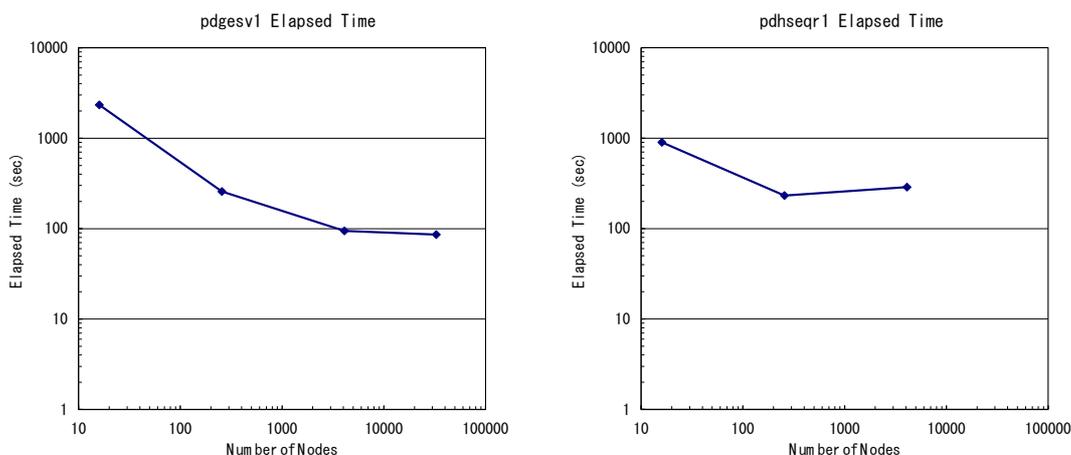
Figure 1: Parallel performance of the ScaLAPACK on the K computer in a strong scaling

(Left: pdgesv, Right: pdhseqr)

Enhancement of the existing OSS

We are also concerned with the demand of a lot of users. There are hundreds of numerical routines of the K computer, which are not implemented but demanded from users strongly. We designed a layer structure of KMATHLIB as shown in Figure 2.
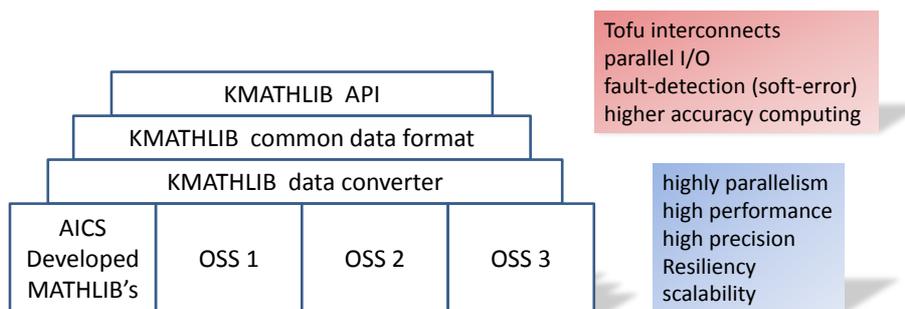
Figure 2: Schematics of the structure of KMATHLIB

We take two ways to develop the KMATHLIB; one is to modify the existing OSS packages, and another is to develop our own solvers to be plugged in the KMATHLIB. On this FY2012-2013, we have modified some of OSS packages and developed following three numerical routines;

➢ The generalized eigenvalues solver taking advantage of Eigen-K,
➢ 3D-decomposition FFT routine, and
➢ Distributed random number generator.

These numerical solvers are quite important tools for scientific simulation codes being studied in AICS.

a) *The generalized eigenvalue solver (KMATH_EIGEN_GEV)* is employed by a lot of simulation code in the material science field. To solve the Schrödinger equation, it yields a nonlinear eigenvalue problem. Then, we modify the non-linear problem to a generalized eigenvalue problem with an iteration scheme, called SCF (Self-Consistent Field calculation). Since, KMATH_EIGEN_GEV is called the innermost loop, thus, it is required to perform very fast. We enhanced our own developed standard eigenvalue solver Eigen-K [1], and implemented it on the K computer. Figure 3 is the parallel performance of the KMATH_EIGEN_GEV routine of the K computer system. It shows the good parallel performance when the number of processes, P (=nodes, here) is composed of large two numbers, for example P is the power of two. The parallel efficiency defined by 'elapsed time using one node' / ('elapsed time using P nodes' * P)

achieves approximately 0.236 (=243.3/16.06*64) when the matrix dimension is 10000 and the number of nodes P=64. Compared with the existing solver, pdsygvx in ScaLAPACK, KMATH_EIGEN_GEV outperforms pdsygvx approximately 1.5 times by the elapsed time when the matrix dimension is 10000 and P=64 (KMATH_EIGEN_GEV→16.06[sec], pdsygvx (NB=32) →23.29[sec]). This implies a big advantage of KMATH_EIGEN_GEV.
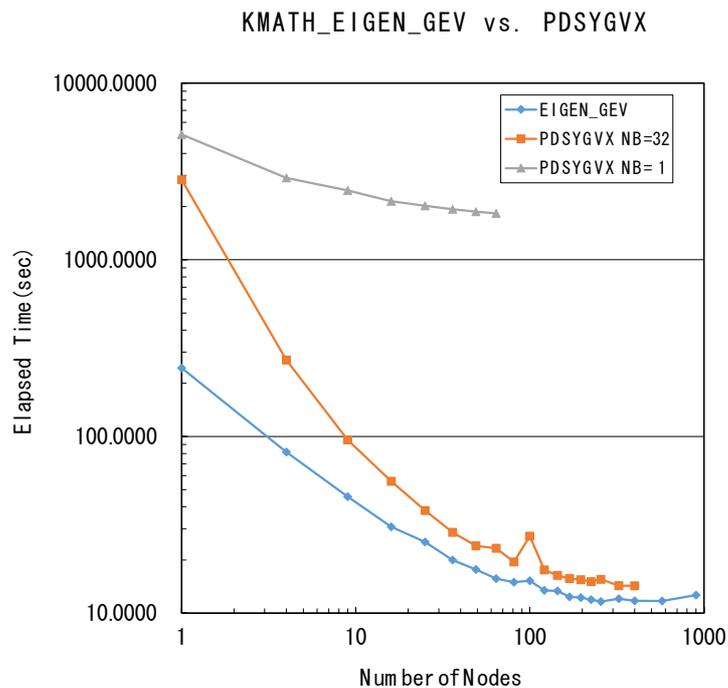
Figure 3: Parallel performance of KMATH_EIGEN_GEV on the K computer in a strong scaling

b) *3D-decomposition FFT routine (KMATH_ FFT3D)* is an innovative enhancement of massively parallel computing in the case that the number of nodes exceeds ten thousand. Current major parallel FFT packages adopt 2D-decomposition data layout, so-called pencil-decomposition. However, it is apparent that the number of parallelism is bounded by the number of grids to be decomposed. When the grid size is assumed to be 100x100x100, 2D-decomposition cannot handle the data on (or map the data into) more than 10000 nodes.

We mainly developed a 3D-decomposition (cubic-decomposition) template program, where user can easily embed and select OSS FFT subroutine such as FFTW [2], FFTE [3], and etc. The call of MPI_Alltoall routines among MPI subcommunications are encapsulated in the implementation.

c) *Random number generator (KMATH_ Random)* is also one of the important numerical tools, as the Monte Carlo simulation plays big role in the scientific simulation codes. Mersenne twister algorithm invented by Prof. Makoto Matsumoto, Hiroshima University, is known as extremely

good random number generator, since it yields a very long period and performs faster. We developed user interface KMATH_Random for the distributed random number generator using dSFMT [4] as a random number engine. KMATH_Random maintains a random seed corresponding to the MPI communicator. Therefore, user can easily generate multiple series of random numbers, flexibly. In addition, the random number period is selectable via an environment variable. For example, in case that "export KMATH_RAND_RANGE=1000" is specified, we obtain a very long period of 2^{1000}.

[1] Eigen-K: http://ccse.jaea.go.jp/ja/download/eigenk.html

[2] FFTW: http://www.fftw.org/

[3] FFTE: http://www.ffte.jp/

[4] dSFMT: http://www.math.sci.hiroshima-u.ac.jp/~m-mat/MT/SFMT/index-jp.html

4.3.2. High precision mathematical library

We have ported a high precision version of PDSYEVD, namely QPEigenK, with the double-double floating point arithmetic data format (hereafter, DD) on a Fujitsu FX10 system which uses a successor microprocessor installed in the K computer. This study is done via joint work with Dr. Susumu Yamada and Dr. Masahiko Machida, Japan Atomic Energy Agency. Figure 4 shows the largest absolute residual error (defined by max |Ax-wx|) on the DD format are plotted with varying matrix dimension. This suggests that the DD version eigenvalue solver offers finer accuracy (approximately 16 digits accurate) than the original SD (single-double) version. Even though the DD format requires additional floating point number operations rather than the SD format, its high accuracy is promising a qualitative improvement large-scale and complex simulations.
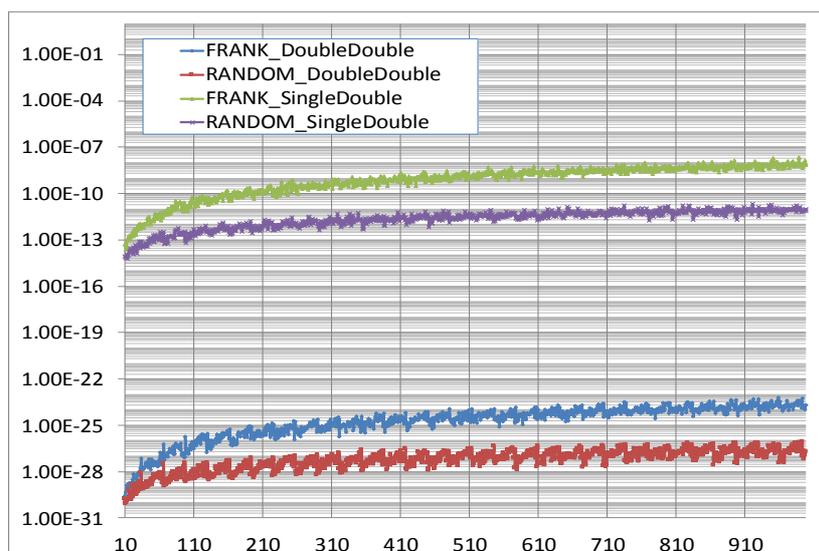
Figure 4: Accuracy test of QPEigenK on a Fujitsu FX10

(Absolute Residual Error max|Ax-wx|_oo)

4.3.3. CREST project

We also studied the high performance and scalable eigenvalue solver supported by the national grant, CREST JST [1] (Program code is "Development of System Software Technologies for post-Peta Scale High Performance Computing"). So far, we have developed the Eigen-K, and performance evaluation and analysis of Eigen-K was carried out on the K computer system. Eigen-K shows good performance scalability and it outperforms representative numerical libraries such as ScaLAPACK [2] and ELPA [3]. Figure 5 presents parallel performance in strong scaling. We examined that Eigen-K and ELPA show a similar tendency of parallel performance while the absolute performance of Eigen-K is two to three times higher. Eigen-K is actually adopted in KMATH_EIGEN_GEV, which is already reported. We can say that performance improvement of KMATH_EIGEN_GEV comes from the big potential of Eigen-K. Through the performance analysis, we recognized that Eigen-K has a severe performance bottleneck in the Divide and Conquer routine which is derived from ScaLAPACK. In future work, we should modify it and remove this performance bottleneck.

[1] http://www.postpeta.jst.go.jp/en/

[2] ScaLAPACK homepage, http://www.netlib.org/scalapack

[3] T. Auckenthaler, V. Blum, H.-J. Bungartz, T. Huckle, R. Johanni, L. Kraemer, B. Lang, H. Lederer, P. R. Willems: Parallel solution of partial symmetric eigenvalue problems from electronic structure calculations, Parallel Computing, Vol. 27, Issue 12, p. 783-794 (2011)
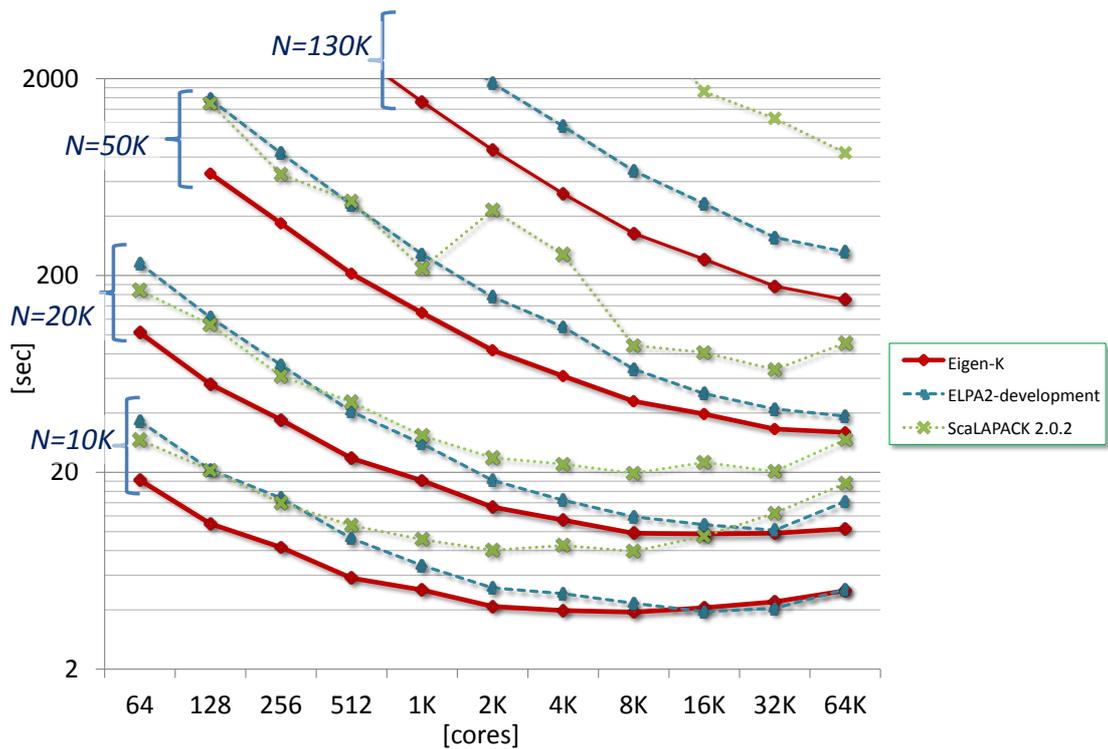
Figure 5: Eigen-K, strong scaling on the K computer

4.4. Schedule and Future Plan

We are developing a software package KMATHLIB which integrates several numerical libraries, such as QPEigenK and Eigen-K. In particular, KMATHLIB will be a prominent result of our primary mission. We plan to release the first version of KMATHLIB at the end of FY2013-2014 as Open Source Software. In addition, the remaining benchmark analysis should be done in the FY2013-2014, and the results will be reflected in the second version of KMATHLIB (the FY2014-2015 or later). We would like to accelerate to integrate OSS packages on the K computer and make it a helpful tool on development of scientific simulation codes.

We still have several key topics not mentioned in this report but to be investigated in the K computer. "Fault tolerance" or "resilience" is one of them. It is well known that FT (fault tolerance) is a big issue not only for the K computer but general peta-scale computer systems. From the viewpoint of the numerical library, we would like to establish the algorithmic fault detection mechanism and its framework, then develop a new type of numerical library taking advantage of such a resilience-aware automatic recovery feature.

4.5. Publication, Presentation and Deliverables

(1) Journal Papers

Currently, not published

(2) Conference Papers

1. <u>T. Imamura</u>, S. Yamada, and M. Machida, "A High Performance SYMV Kernel on a Fermi-core GPU", High Performance Computing for Computational Science - VECPAR 2012, Lecture Note in Computer Science (LNCS) 7851, pp.59-71, 2013.

(3) Invited Talks

   -None

(4) Posters and presentations

1. <u>T. Imamura</u>, S. Yamada, M. Machida, "Preliminary Report for a High Precision Distributed Memory Parallel Eigenvalue Solver", The International Conference for High Performance Computing, Networking, Storage and Analysis (SC12), poster presentation, Salt Lake City, US. Nov. 2012.

2. Y. Idomura, M. Nakata, S.Yamada, <u>T. Imamura</u>, T. Watanabe, M. Machida, M. Nunami, H. Inoue, S. Tsutsumi, I. Miyoshi, N. Shida, "Communication Overlap Techniques for Improved Strong Scaling of Gyrokinetic Eulerian Code Beyond 100k Cores on K-Computer", The International Conference for High Performance Computing, Networking, Storage and Analysis (SC12), poster presentation, Salt Lake City, US. Nov. 2012.

3. <u>T. Imamura</u>, S. Yamada, M. Machida, "Eigen-K: high performance eigenvalue solver for symmetric matrices developed for K computer", 7th International Workshop on. Parallel Matrix Algorithms and Applications (PMAA2012), June 2012, London UK. June 2012.

4. T. Imamura, "Performance Auto-Tuning in Memory-Bound CUDA-BLAS Kernel", 2013 @square HPSC, Conference on Advanced Topics and Auto Tuning in High Performance Scientific Computing, National Taiwan University, Taipei, Taiwan, 27-29 March 2013.

5. T. Imamura, "Beyond Peta-scale Computing from the Viewpoint of Numerical Libraries", The 3rd AICS International Symposium, Computer and Computational Science for Exascale Computing, RIKEN AICS, Kobe, Japan, 28 Feb.-1 March 2013.

6. <u>T. Imamura</u>, T. Utsumi, X. Lin, S. Yamada, and M. Machida, "Performance Tuning for the SYMV kernel on multiple GPU generations, Fermi and Kepler", IPSJ SIG Technical Reports, Vol.2012-HPC-138, No.8, pp.1-7, 2013-02-14. (Japanese).

7. T. Imamura, "KMATHLIB: development of a numerical library on the K computer", The 5-th HPCI Strategic Program Joint research exchange meeting, RIKEN AICS, Kobe, Japan, Jan.

2013.

8. S. Yamada, N. Sasa, <u>T. Imamura</u>, and M. Machida "Quadrature Precision Basic Linear Algebra Subprograms and Its Applications", IPSJ SIG Technical Reports, Vol.2012-HPC-137, No.23, pp.1-6, Dec. 2012. (Japanese)

9. T. Imamura, "Development of a numerical library on the K computer", Workshop on Applied and Computational Mathematics in Industry, Tokyo, Japan, Dec. 2012.

10. <u>T. Imamura,</u> S. Yamada, and M. Machida, "Prospective figure of an Eigensolver for a Dense matrix in an emerging post peta-scale computing Era", JSIAM annual meeting 2012, Wakkanai, Japan, Aug. 2012.

11. S. Yamada, Y. Idomura, <u>T. Imamura</u>, and M. Machida, "Convergence property of Krylov subspace methods for system of linear equations on fusion plasma simulation code GT5D", JSIAM annual meeting 2012, Wakkanai, Japan, Aug. 2012.

12. <u>T. Imamura</u>，T. Yoshida，R. Tamura，H. Kondo，S. Yamada，and M. Machida, "High Performance eigenvalue solver accelerated with an auto-tunner mechanism concering with multicore communication hiding", IPSJ SIG Technical Reports, Vol.2012-HPC-135, No.19, pp.1-8, July 2012. (Japanese)

13. <u>T. Imamura</u>, S. Yamada, and M. Machida, "Eigen-Exa: development of the eigensolver for dense matrices on a post peta-scale computing environment", JSCES annual meeting 2012, Kyoto, Japan, May 2012.

(5) Patents and Deliverables
Currently None

5. HPC Usability Research Team

5.1. Team members

Toshiyuki Maeda (Team Leader)

Yoshiki Nishikawa (Visiting Researcher)

Akiko Yoshioka (Assistant)

5.2. 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. Software verification

   Software 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.

5.3. Research Results and Achievements

5.3.1. Protocol/API Design for Computing Portal Framework

As a first step of designing and implementing a computing portal framework that can be used by wide range of users, in FY 2012, we designed an experimental API/protocol for computing services. More specifically, we designed APIs/protocols that handle registration of services and their providers, registration and authentication of users for each registered service, invocation of computing services, data sharing among multiple computing services, and so on.

The APIs/protocols are designed in such a way to work with the current popular web-based application frameworks (e.g., HTTP, JSON, etc.). Therefore, in theory, we can write programs that utilize multiple computing services in various programming languages (e.g., Ruby, Python, JavaScript, etc.). In addition, a computing service can be registered and published by writing a simple XML file, provided that the application programs of the computing service are installed on the backend system. Based on the experimental API/protocol, we are also implementing a prototype system that can be used to publish existing applications as computing services.

One limitation of the designed experimental APIs/protocols and their prototype implementation is that security mechanisms are not fully integrated or realized yet. That is, malicious computing services can access data of other computer services, and/or leak data of one user to another user. To address the problem, we are planning to improve the APIs/protocols from the viewpoint of security and enhance the prototype implementation by integrating virtualization techniques.

5.3.2. Virtualization Techniques

1. Lightweight virtualization for testing/debugging parallel programs

    In order to utilize the full power of today's HPC systems as the K computer, users have to write massively parallel programs. However, writing parallel programs is difficult compared to conventional sequential programming. This is because parallel programs have inherent non-determinacy (e.g., process/thread execution order), that is, even if a parallel program contains a bug, it is not always easy to reproduce the bug. In addition, performance bottlenecks

of parallel programs are not apparent from their source code because network latency, synchronization costs, scalability, etc. cannot be inferred directly from the source code. One possible solution to the problems is to utilize static source code analysis and dynamic performance profiling, however, some kind of bugs arise only when the number of processes/threads used by parallel programs is huge (e.g., several tens of thousands or more).

In order to address the above mentioned problem, in FY 2012, we designed a lightweight network virtualization technique that is useful for testing/debugging parallel programs. More specifically, we designed a virtualization framework that is able to provide several tens to hundreds of virtual execution environments per real (physical) execution environment. With the virtualization framework, users can test, debug, and/or profile their parallel programs on a limited number of physical computing nodes as if the programs run on a huge number of nodes.

The key of our virtualization framework is to virtualize network related operations at the level of shared libraries. Current popular virtualization technologies adopt virtualization at the level of CPU (with hardware assists) or OS (system calls), which is heavier than the level of shared libraries. This is because main purpose of the popular virtualization technologies is to provide virtual execution environments that are hard to be distinguished from real (physical) ones. Our virtualization framework, on the other hand, gives up to provide such a realistic virtual execution environment, but instead aims to provide as much as possible of virtual execution environments per real (physical) one. By adopting virtualization at the level of shared libraries, the performance overheads of hooking system calls and/or CPU events (e.g., interrupts and exceptions) can be eliminated (while statically linked programs, that is, programs do not rely on shared libraries, will not be virtualized correctly).

In addition, our virtualization framework tries to reduce (or eliminate) exchange of virtual network routing information among real (physical) nodes. In order to correctly route packets from one virtual execution environment to another, all the physical nodes have to share the routing information of the virtual networks because the virtual execution environments may reside in different physical nodes. Therefore, if a single physical node manages the routing information, the node will become a performance bottleneck because all the other physical nodes have to synchronize with the node each time they need to route packets.

To address the problem, our virtualization framework tries to distribute the routing information statically (that is, before executing programs in virtual execution environments) as much as possible. In addition, even if dynamic updating of the routing information is inevitable, our virtualization framework tries to minimize synchronization between multiple physical nodes by separating allocation pool of physical (real) network ports statically.

Based on the above mentioned design, we are also implementing its prototype system, and will continue the development in FY 2013.

2. CPU emulator for SPARC 64 VIIIfx

One problem of the current K computer is that its CPU is based on the SPARC 64 VIIIfx architecture, which is not so popular in the current PC market dominated by the x86-64 architecture. Therefore, users have to use a cross compiler which generates SPARC binaries on the front-end node of the K computer, or their x86-64 PCs. Thus, it is somewhat difficult to develop software for the K computer because programmers cannot test their programs on their ordinary development environment (e.g., PCs), and have to use the K computer even if they want to conduct very small tests.

To address the problem, we are implementing a CPU emulator for SPARC 64 VIIIfx. A CPU emulator is a program that emulates behavior of a CPU architecture that is different from that of the host machine on which the emulator itself runs. Our CPU emulator is able to execute SPARC 64 VIIIfx executables on ordinary x86-64 PCs. More specifically, we modified the existing CPU emulator QEMU to support the features specific to the SPARC 64 VIIIfx architecture (e.g., extended general purpose/floating-pointer registers, SIMD extension, etc.).

In FY 2012, we developed a rapid prototype of our CPU emulator. The prototype only supports a subset of the SPARC 64 VIIIfx architecture and very small number of system calls. Moreover, its emulation is incomplete in the sense that it does not adhere to the formal specification of SPARC 64 VIIIfx and sometimes crashes abnormally. We are planning to develop a more stable and faithful prototype which is usable for practical program development and testing in FY 2013.

5.3.3. Software Model Checking for Partitioned Global Address Space Language (Joint Work with Programming Environment Research Team)

Partitioned Global Address Space Languages (or, PGAS languages) are programming languages for distributed computing systems where the systems consist of large number of computing nodes and their memories are distributed among the nodes. In the PGAS languages, all the processes and/or threads in a program can share a single address space even though the memories are distributed, as in traditional distributed shared memory (DSM) systems. One of the distinguishing features of the PGAS languages is that the shared address space can be partitioned into sub-spaces and they can be bound to a specific process and/or thread explicitly. Thus, programmers can write a locality-aware program which is essential to achieve high performance on massively-parallel distributed memory systems of today (and future).

Despite the above mentioned advantage, one big problem with PGAS languages is that programmers can easily introduce concurrency bugs. For example, if multiple threads access a portion of a single address space simultaneously without proper synchronizations, race condition bugs can be easily introduced even if the accessed portion is bound to a specific process and/or

thread. To make things worse, introducing synchronizations is not as easy as it sounds because excessive use of synchronizations severely degrades performance, while lack of them introduces hard-to-debug and non-reproducible concurrency bugs.

To address the problem, in FY 2012, we proposed and implemented a software model checking framework for PGAS languages. Software model checking is a program verification approach which tries to prove that a given program satisfies a certain property by exploring all the program states that can be reached during program execution. One problem of model checking PGAS programs is that it tends to suffer from the state explosion problem because these programs allow concurrent and/or parallel execution and memory sharing. To avoid this problem, it is essential to perform proper abstractions based on the properties to be verified because they can dramatically reduce the number of states to be explored. However, it is not always easy to automatically infer proper abstractions because programs and properties to be verified vary.

To address the state explosion problem, we proposed a model checking framework that includes user-definable abstractions. The key idea of the framework is that it exposes the intermediate representation of the program's abstract syntax tree, enabling users to define their own abstractions flexibly and concisely by creating a translator to translate the trees. We also implemented CAF-SPIN, our proof-of-concept prototype of a model checking tool for Coarray Fortran. The experimental results with CAF-SPIN showed that abstractions can be defined easily and concisely by users, and the number of states to be explored for model checking is dramatically reduced with the abstractions.

Moreover, we also implemented XMP-SPIN, our software model checking tool for XcalableMP (http://www.xcalablemp.org/), and conducted several experiments with XMP-SPIN. More specifically, we conducted model checking of a number of parallel stencil computations written in XcalableMP (from small test programs to large application programs). Although stencil computations offer a simple and powerful programming style in parallel programming, they are sometimes error prone when considering optimization and parallelization because optimization of stencil computation may involve complex loop transformations and/or array reindexing, and parallelization requires explicit communication (data synchronizations) among multiple processes. In the experiments with XMP-SPIN, we checked whether there are no missing or redundant data synchronizations in the target programs, and successfully found four bugs in a reasonable time with a reasonable amount of memory.

5.4. Schedule and Future Plan

In FY 2013, we will improve the APIs/protocols for our computing portal framework designed in FY 2012 from the viewpoint of security. As mentioned above, the current experimental

APIs/protocols and their prototype implementation do not consider security mechanisms seriously. Therefore, malicious computing services can access data of other computer services, and/or leak data of one user to another user. In addition to the improvement of the API/protocols, we will also improve and enhance the prototype implementation by integrating virtualization techniques.

Regarding the virtualization technologies, we will continue to implement the lightweight network virtualization framework for testing/debugging parallel programs and the CPU emulator for SPARC 64 VIIIfx for running binary executables for the K computer on the ordinary x86-64 computers.

Regarding the software verification, we will conduct more experiments with CAF-SPIN and XMP-SPIN to evaluate their effectiveness and practicality. In addition, we will also consider applying our software model checking approach to other PGAS languages. Moreover, we will also plan to extend our model checking approach to take into consideration relaxed memory consistency models.

As a slightly longer-term goal, we plan to start integrating the research results of the virtualization technologies and the software verification into the computing portal somewhere from the second half of FY 2014 to the first half of FY 2015.

5.5. Publication, Presentation and Deliverables

(1) Conference proceedings (Refereed)

1. Tatsuya Abe, Toshiyuki Maeda, and Mitsuhisa Sato. Model checking with user-definable abstraction for partitioned global address space languages. In Proceedings of the 6th Conference on Partitioned Global Address Space Programming Models (PGAS2012), Online. Santa Barbara, October 2012.

2. Tatsuya Abe, Toshiyuki Maeda, and Mitsuhisa Sato. Model checking stencil computations written in a partitioned global address space language. In Proceedings of the 18th International Workshop on High-Level Parallel Programming Models and Supportive Environments (HIPS2013), to appear.

(2) Presentations

1. Toshiyuki Maeda. Brief introduction of HPC usability research team. The 3rd AICS International Symposium, March 2013.

(3) Deliverables

1. CAF-SPIN: A software model checker for Coarray Fortran (in preparation for release)

(4)   Posters and presentations

　　-None

(5) Patents and Deliverables

     -None

6. Field Theory Research Team

6.1. 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)

Ken-Ichi Ishikawa (Visiting Scientist)

Shinji Takeda (Visiting Scientist)

Takeshi Yamazaki (Visiting Scientist)

6.2. 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.

6.3. Research Results and Achievements

6.3.1. 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. The Monte Carlo simulation technique, which has been successfully applied to the finite temperature phase transition studies in lattice QCD, cannot be directly applied to the finite density case due to the complexity of the quark determinant for finite μ. Recently we investigated the phase of the quark determinant with finite chemical potential in lattice QCD using an analytic method: Employing the winding expansion and the hopping parameter expansion to the logarithm of the determinant, we have shown that the absolute value of the phase has an upper bound that grows with the spatial volume but decreases exponentially with an increase in the temporal extent of the lattice. Based on this analysis we have carried out a finite size scaling study for 4 flavor QCD using the O(a) improved Wilson quark action and the Iwasaki gauge action. This is the first application of the finite size scaling study to the finite density QCD. We choose κ =0.1385 at β =1.58 whose lattice spacing is roughly 0.33 fm. Spatial volume is varied from 6^3 to 10^3 with the temporal size fixed at N_T=4. The transition point is around μ /T〜0.5. The left panel of Fig. 1 shows the susceptibility of the quark number as a function of a μ. We observe that the peak height grows as the spatial volume increases. In the right panel of Fig. 1 we plot the spatial volume dependence of the susceptibility peak for various obsevables including the quark number. A clear linear scaling indicates the first order phase transition. These are encouraging results demonstrating that the finite size scaling study is useful even in the finite density QCD.
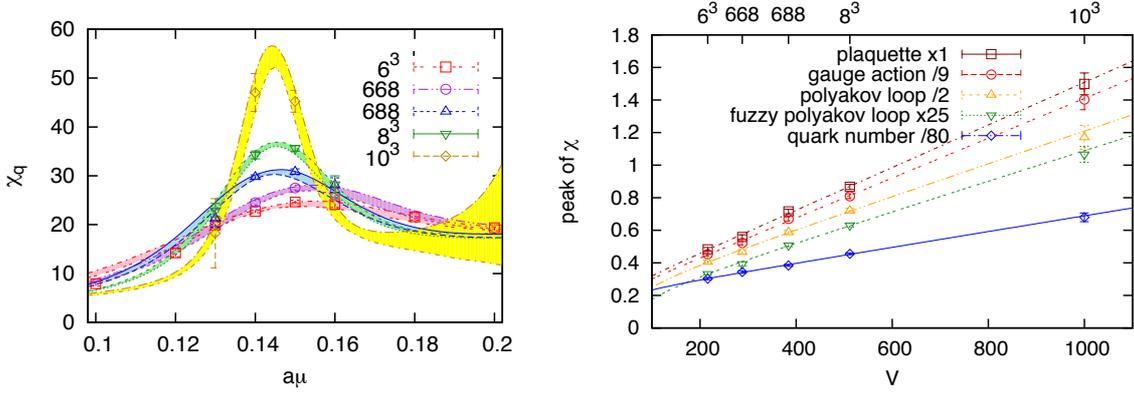
Figure 1: Susceptibility of the quark number as a function of a μ (left) and spatial volume dependence for various observables together with the fit results in the form of $c_1 V + c_0 + c_{-1}/V$ with V the spatial volume (right).

6.3.2 Nuclei in lattice QCD

In 2010 we succeeded in a direct construction of the ^{4}He and ^{3}He nuclei from quarks and gluons in lattice QCD for the first time. Calculations were carried out at a rather heavy degenerate up- and down-quark mass corresponding to m_π=0.8 GeV in quenched QCD to control statistical errors in the Monte Carlo evaluation of the helium Green's functions. As a next step we have investigated the dynamical quark effects on the binding energies of the helium nuclei, the deuteron and the dineutron. We perform 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. In Fig. 2 we plot the spatial volume dependence of the energy difference ΔE_L as a function $1/L^3$ with L the spatial extent. A finite energy difference left in the infinite spatial volume limit leads us to the conclusion that the measured ground states for all the channels are bound. We also point out a possibility that the dynamical quark effects might be small at rather heavy quark mass region.
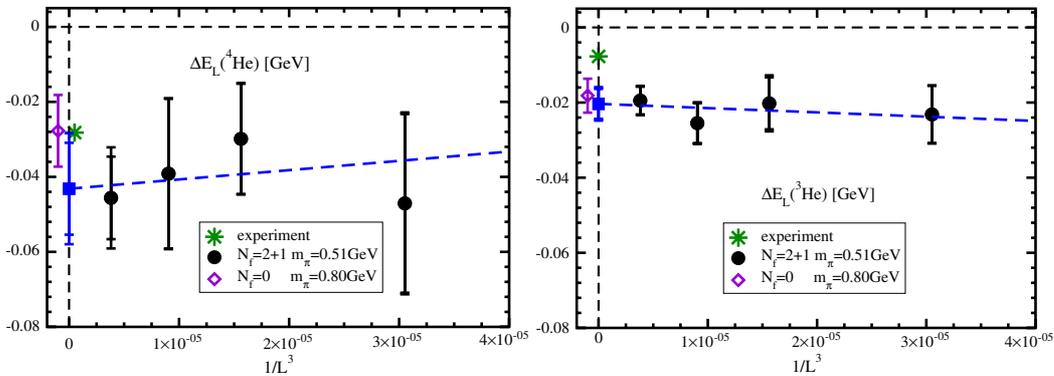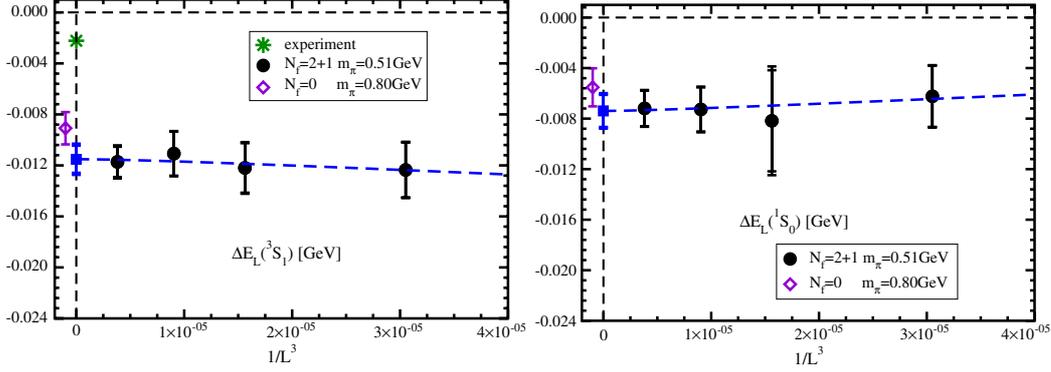
Figure 2: Spatial volume dependence of ΔE_L in GeV units for the ^{4}He (top left), ^{3}He (top right), ^{3}S$_1$ (bottom left) and ^{1}S$_0$ (bottom right) channels. Extrapolated results to the infinite spatial volume limit in 2+1 flavor QCD (blue square) and quenched QCD (violet diamond) are also presented.

6.3.3. Development of algorithms and computational techniques

We consider to solve the linear systems with multiple right-hand sides expressed as AX=B, where A is an N×N matrix and X, B are N×L matrices with L the number of multiple right-hand side vectors. Various fields in computational sciences face this type of problem. In lattice QCD simulations, for example, one of the most time consuming part is to solve the Wilson-Dirac equation with the multiple right-hand sides, where A is an N×N complex sparse non-Hermitian matrix and X, B are N×L complex matrices with N the number of four dimensional space-time sites multiplied by 12. We aim at reducing the computational cost with the block Krylov subspace method which makes convergence faster than the non-blocked method with the aid of better search vectors generated from wider Krylov subspace enlarged by the number of multiple right-hand side vectors. We improve the block BiCGSTAB algorithm with the QR decomposition. After an optimization of the matrix-vector multiplication on K computer, the sustained performance for the block solver has reached nearly 35% of theoretical peak performance.

6.4. Schedule and Future Plan

6.4.1. QCD at finite temperature and finite density

Before exploring the phase structure in 2+1 flavor QCD, we plan to investigate the 3 flavor case with the finite size scaling study. We mainly focus on the location of the critical end line in three dimensional parameter space of the pion mass, chemical potential and temperature.

6.4.2. Nuclei in lattice QCD

The existence of the bound state observed in the $^1S_0$ channel in 2+1 flavor QCD looks odd from the experimental point of view. We expect that the bound state in the $^1S_0$ channel vanishes at some lighter quark mass toward the physical point. To confirm this scenario we are now carrying out a simulation around m_π=300 MeV in 2+1 flavor QCD.

6.4.3. Development of algorithms and computational techniques

We are now ready to check the arithmetic performance and the scalability of the block BiCGSTAB with the QR decomposition optimized on K computer employing a real problem in lattice QCD. We investigate to what extent the cost is reduced thanks to diminished number of iterations and efficient cache usage.

6.5. Publication, Presentation and Deliverables

(1) Journal Papers

1. PACS-CS Collaboration: S. Aoki et al., 1+1+1 Flavor QCD+QED Simulation at the Physical Point", Physical Review D86 (2012) 034507.

2. T. Yamazaki, K.-I. Ishikawa, Y. Kuramashi, A. Ukawa, "Helium nuclei, deuteron and dineutron in 2+1 flavor lattice QCD", Physical Review D86 (2012) 074514.

3. Tuomas Karavirta, Jarno Rantaharju, Kari Rummukainen, Kimmo Tuominen, "Determining the conformal window: SU(2) gauge theory with N_f= 4, 6 and 10 fermion flavours", Journal of High Energy Physics 1205 (2012) 003.

(2) Conference Papers

1. H. Suno, E. Hiyama, M. Kamimura, "Theoretical study of triatomic systems involving helium atoms", (Accepted, talk given at the 20th International IUPAP Conference on Few-Body Problems in Physics (Fukuoka, Japan, August 20-24, 2012)).

2. X.-Y. Jin and R. D. Mawhinney, "Lattice QCD with 12 Quark Flavors: A Careful Scrutiny", (Accepted, talk given at Strong Coupling Gauge Theories in the LHC Perspective (SCGT 12) (Nagoya University, Nagoya, Japan, December 4-7, 2012)).

3. Tuomas Karavirta, Kimmo tuominen, Jarno Rantaharju, Kari Rummukainen, "Mapping the Conformal Window: SU(2) with 4, 6 and 10 flavors of fermions", Proceedings of Science LATTICE2012 (2012) 037.

4. T. Boku, K.-I. Ishikawa, Y. Kuramashi, K. Minami, Y. Nakamura, F. Shoji, D. Takahashi, M. Terai, A. Ukawa, T. Yoshie, "Multi-block/multi-core SSOR preconditioner for the QCD quark solver for K computer", Proceedings of Science (Lattice 2012) 188.

5. T. Yamazaki, K.-I. Ishikawa, Y. Kuramashi, A. Ukawa, "Bound states of multi-nucleon

channels in N_f=2+1 lattice QCD", Proceedings of Science (Lattice 2012) 143.

6. S. Takeda, X-Y. Jin, Y. Kuramashi, Y. Nakamura, A. Ukawa, "Finite size scaling for 4-flavor QCD with finite chemical potential", Proceedings of Science (Lattice 2012) 066.

(3) Invited Talks

1. Yoshinobu Kuramashi, "1+1+1 Flavor QCD+QED Simulation at the Physical Point", New Horizons for Lattice Computations with Chiral Fermions (BNL, New York, USA, May 14-16, 2012).

2. Yoshinobu Kuramashi, "Lattice QCD – From Quarks and Nuclei –", 10th International Meeting on High-Performance Computing for Computational Science (VECPAR2012) (Kobe, Japan, July 17-20, 2012).

3. Yoshifumi Nakamura, "Block Krylov Subspace Method for QCD Simulation", QCDNA VII (University of Adelaide, Adelaide, Australia, July 2-4, 2012).

4. H. Suno, "Efimov effect and resonances in atomic and molecular physics", YITP workshop: Resonances and non-Hermitian systems in quantum mechanics (Kyoto, Japan, December 13-16, 2012).

5. X.-Y. Jin and R. D. Mawhinney, "Lattice QCD with 12 Quark Flavors: A Careful Scrutiny", Strong Coupling Gauge Theories in the LHC Perspective (SCGT 12) (Nagoya University, Nagoya, Japan, December 4-7, 2012).

6. X.-Y. Jin and R. D. Mawhinney, "Exploring the phases of QCD with many flavors", QCD Structure I (Central China Normal University, Wuhan, China, October 7-20, 2012).

7. X.-Y. Jin and R. D. Mawhinney, "Exploring the phases of QCD with many flavors", New Horizons for Lattice Computations with Chiral Fermions (BNL, New York, USA, May 14-16, 2012).

8. Jarno Rantaharju, "Mapping Conformal Field theories on the Lattice", Final Colloquium, International Research Training Group, GRK 881, Paris - Bielefeld - Helsinki (Bielefeld University, Germany, September 12 - 14, 2012).

9. Takeshi Yamazaki, "Light nuclei from quenched lattice QCD", New Horizons for Lattice Computations with Chiral Fermions (Brookhaven National Laboratory, NY, USA, May 14-16, 2012).

10. Takeshi Yamazaki, "Calculation of light nuclei from N_f=2+1 lattice QCD", Lattice Hadron Physics IV (LHP IV) (University of Adelaide, Adelaide, Australia, July 2-4, 2012).

11. Takeshi Yamazaki, "Calculation of light nuclei from N_f=2+1 lattice QCD", Cross over workshop "Particle, nucleus, and Universe" x "New Hadron" (Nagoya University, Nagoya, July 12-13, 2012).

12. Takeshi Yamazaki, "Calculation of light nuclei from lattice QCD", Quarks to Universe in

Computational Science (QUCS 2012) (the Reception Hall in Nara Prefectural New Public Hall, Nara, December 13-16, 2012).

13. Takeshi Yamazaki, "Calculation of light nuclei from N_f=2+1 lattice QCD", HPCI Field 5 meeting (FUJISOFT AKIBA Plaza, Tokyo, March 5-6, 2013).

14. Shinji Takeda, "Complex phase of quark determinant of QCD with finite chemical potential and phase structure of 4-flavor QCD", Tokyo Institute of Technology Theoretical Nuclear Physics group Seminar (Ookayama, Tokyo, September 27, 2012).

(4)　Posters and presentations

1. Yoshifumi Nakamura, "Towards high performance Lattice QCD simulations on Exascale computers", SC12 (Salt Lake City, Utah, USA, November 10-16, 2012).

2. Yoshifumi Nakamura, "Towards high performance Lattice QCD simulations on Exascale computers", The 3rd AICS International Symposium (Kobe, Japan, February 28 - March 1, 2013).

3. H. Suno, Y. Nakamura, K.-I. Ishikawa, Y. Kuramashi, "Modified Block BiCGSTAB for Lattice QCD on K Computer", The 3rd AICS International Symposium (Kobe, Japan, February 28 - March 1, 2013).

4. H. Suno, E. Hiyama, M. Kamimura, "Theoretical study of triatomic systems involving helium atoms", The 20th International IUPAP Conference on Few-Body Problems in Physics (Fukuoka, Japan, August 20-24, 2012).

5. H. Suno, E. Hiyama, M. Kamimura, "Theoretical study of triatomic systems involving helium atoms" , The 2012 Annual Meeting of Physical Society of Japan (Yokohama, Japan, September 18-21, 2012).

6. H. Suno, E. Hiyama, "Application of the gaussian expansion method to cold atomic few-body systems" , Quarks to Universe in Computational Science (Nara, Japan, December 13-15, 2012).

7. X.-Y. Jin, S. Takeda, Y. Kuramashi, Y. Nakamura, A. Ukawa, "Studying Quantum Chromodynamics at Finite Temperature and Density", The 3rd AICS International Symposium (Kobe, Japan, February 28 - March 1, 2013).

8. X.-Y. Jin, S. Takeda, Y. Kuramashi, Y. Nakamura, A. Ukawa, "Reweighting and Lee-Yang Zero", The 30th International Symposium on Lattice Field Theory (Cairns Convention Centre, Cairns, Australia, June 24-29, 2012).

9. Jarno Rantaharju, Kari Rummukainen, Kimmo Tuominen, "Running coupling in SU(2) with adjoint fermions", Strong Coupling Gauge Theories in the LHC Perspective (SCGT 12), (Nagoya University, Nagoya, Japan, December 4 - 7, 2012).

10. Jarno Rantaharju, Kari Rummukainen, Kimmo Tuominen, "Running coupling in SU(2) with

adjoint fermions", The 3rd AICS International Symposium (Kobe, Japan, February 28 - March 1, 2013).

11. Takeshi Yamazaki, Y. Kuramashi, A. Ukawa, "Bound states of multi-nucleon channels in N_f=2+1 lattice QCD", The 30th International Symposium on Lattice Field Theory (Lattice 2012) (Cairns Convention Centre, Cairns, Australia, June 24-29, 2012).

12. Takeshi Yamazaki, Y. Kuramashi, A. Ukawa, "Study of multi-nucleon bound states from N_f=2+1 lattice QCD", JPS autumn meeting (Kyoto Sangyo University, Kyoto, September 11-14, 2012).

13. Shinji Takeda, "Finite size scaling for 4-flavor QCD with finite chemical potential", The 30th International Symposium on Lattice Field Theory, Lattice 2012 (Cairns Convention Centere, Cairns, Australia, June 24-29, 2012).

14. Shinji Takeda, "Finite size scaling for 4-flavor QCD with finite chemical potential", New Frontiers in Lattice Gauge Theory (The Galileo Galilei Institute for Theoretical Physics, Florence, Italy, August 28-September 28, 2012).

(5) Patents and Deliverables
    -None

7. Discrete Event Simulation Research Team

7.1. Team members

Nobuyasu Ito (Team Leader)

Hajime Inaoka (Research Scientist)

Tetsuo Imai(Postdoctoral Researcher)

7.2. Research Activities

This team started on October 1st in 2012, and preparation to start up the team were conducted in this year. Four team members were designated: two joined the team in the end of fiscal year of 2012(Dr. Inaoka from February 2013, and Dr. Imai from March 2013). Two more will join in April 2013. Cluster server and workstations for the team were procured are started operation.

7.3. Research Results and Achievements

Research results and achievements will come in the following years.

7.4. Schedule and Future Plan

During the following years, this team will develop software for discrete-event simulation for K computer and study their application for social phenomena. Two kinds of applications will be studied and developed: one is simulation software for graph simulations, and the other is management software for various application software with various parameters.

The first one for graph software is to simulate graph dynamics and dynamics on graph. Graphs are discrete objects characterize heterogeneous structures which are ubiquitously observed in discrete-event phenomena, for example, traffic networks, human relations and economic activity. Simulations of those discrete-event phenomena need to treat evolutions on given graphs, for example, how cars flow on roads, and also to treat development of graph structures, for example, how new roads and highways are constructed and destroyed.

However, high-performance computers nowadays are desined for homogeneous simulations, for example, number crunching ones on regular lattices or with regular structures. Graph treatment is still underdeveloped stage. This team has started to develop such graph treatment on K computer, and simulation software for various discrete-event phenomena will be studied and developed.

In general, discrete-event simulations are accompanied with combinatorial variety of input and output. For example, a small change in control of traffic signal may cause disastrous jam. Smooth output cannot be expected from a small change in input. Combinatorial effort for parameter search and output fitting for various simulation models will be necessary. The other kind of applications, management software, is to enable to attack this challenge beyond human brains and hand works.

Preliminary version of graph treatment software and management software will be developed and tested in 2013. Application software for some basic social simulations, for example, traffic flow, human crowd, economic trade and human relations will be developed in 2014 and 2015. Those will work with the management software. In 2016 and 2017, those software will be released for K computer users.

7.5. Publication, Presentation and Deliverables

(1) Journal Papers

Koji Oishi, Takashi Shimada and Nobuyasu Ito, " Group Formation through Indirect Reciprocity," Physical Review E vol.87 (2013) p.030801(R)(4 pages).

(2) Conference Papers
   -None

(3) Invited Talks
   -None

(4) Posters and presentations
   1. 26th Workshop "Recent Developments in Computer Simulation Studies in Condensed Matter Physics" (The University of Georgia, Athens, U.~S.~A., February 25-29, 2013)
   2. Nobuyasu Ito, "Human behavior in video sharing sites".
   3. Koji Oishi and Nobuyasu Ito, "Group Formation through Indirect Reciprocity".

(5) Patents and Deliverables
   -None

8. Computational Molecular Science Research Team

8.1. Team members

Takahito Nakajima (Team Leader)

Tomomi Shimazaki (Research Scientist)

Yoshinobu Akinaga (Research Scientist)

Michio Katouda (Postdoctoral Researcher)

Yutaka Nakatsuka (Postdoctoral Researcher)

Yusuke Ootani (Postdoctoral Researcher)

Toru Matsui (Visiting Researcher)

Muneaki Kamiya (Visiting Researcher)

8.2. Research Activities

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

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

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

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

To achieve our aim, we have so far developed several methods of calculation. Examples include a way for resolving a significant problem facing conventional methods of calculation, in which the calculation volume increases dramatically when dealing with larger molecules; a way for improving the precision of calculations in molecular simulations; and a way for high-precision calculation of the properties of molecules containing heavy atoms such as metal atoms. We have integrated these calculation methods into a software package named NTChem that we are developing, which can run on the K computer and which contains a variety of high-performance calculation methods and functions. By selecting and combining appropriate methods, researchers can

perform calculations suitable for their purpose. For example, it is possible to obtain a rough prediction of the properties of a molecule in a short period of time, or obtain a precise prediction by selecting a longer simulation. In addition, NTChem is designed for high performance on a computer with many compute nodes (high concurrency), and so it makes optimum use of the K computer's processing power.

8.3. Research Results and Achievements

8.3.1. Massively parallel second-order Møller–Plesset perturbation calculations on K computer

Second-order Møller–Plesset perturbation theory (MP2) is the simplest method to account for electron correlation at ab initio level. However, the computational costs of conventional MP2 are considerably high and its practical applications are limited. For MP2 calculations the development of efficient computational techniques is important. Last year, we developed a MPI/OpenMP hybrid parallel algorithm for the massively parallel computations of resolution-of-identity MP2 (RI-MP2) method. This algorithm works efficiently on commodity supercomputers such as Riken RICC massively parallel PC cluster system. In this year, we have developed a incore algorithm suitable for the massively parallel computations on K computer. In this algorithm, the disk storage of intermediate data was replaced with memory storage to avoid the I/O overhead of accessing local scratch areas in K computer. We have implemented this new incore and MPI/OpenMP parallel RI-MP2 algorithm into NTChem quantum chemistry software developed in our team. The new implementation has been supplied as a library software on K computer. Using the new RI-MP2 codes, MP2 calculations of large molecules having up to 300 atoms and 7000 atomic orbitals can be performed with high parallel performance and in modest times on K computer. We successfully performed the RI-MP2/cc-pVTZ calculation of π-π stacked two-layer nanographene sheets $(C_{96}H_{24})_2$ (6432 atomic orbitals) on K computer. The calculation was finished in 33 minutes using 2048 node and 16384 CPU cores of K computer. Using the new RI-MP2 codes, MP2 calculations of large molecules with up to 500 atoms can be performed in modest times on K computer. We have been developing the parallel RI-MP2 analytical energy gradient program enable to perform the geometry optimization calculations of molecules with about 500 atoms and ab initio molecular dynamic simulations of molecules with about 100 atoms on K computer.

8.3.2. Development of two-component relativistic coupled-cluster programs

Consideration of relativity in molecular quantum-chemical calculations is one of the most important factors for heavy-element systems. In the last financial year we developed general-order spin-free and two-component relativistic spin–orbit coupled-cluster (SOCC) programs for ground-

and excited-state correlation energies with the aid of an automatic code-generation technique. The developed generator program derives algebraic CC equations automatically for a given order, factorizes the terms in each equation, and generates Fortran programs for solving the equations. The development in this period includes (1) improvement of the generator such that level 3 BLAS routines are employed in tensor multiplications, (2) automatic algebraic derivation and solution of Lambda equations which are the key equations for computing coupled-cluster ground-state electronic properties, and (3) computation of ionization potentials through diagonalization of CC Jacobian. Excellent agreement was obtained between the calculated results using our programs and experiment for the ionization spectrum of an OsO_4 molecule, which is known to exhibit a well-known splitting due to spin-orbit interaction. The program was also tested for spin–orbit splittings of excited states of atoms and excitation energies of a TlH molecule, showing satisfactory agreements with the literature. The directions in the next financial year are: (1) large-scale parallelization and (2) development of analytical energy gradients for ground and excited states.

8.3.3. Development of analytical energy gradient for time-dependent density functional theory

Precise information on excited state potential energy surfaces is the most important prerequisite for a deeper understanding of photochemical reaction or the shape of absorption and luminescence spectra. The development and efficient implementation of an analytic gradient theory for reliable theoretical models incorporating electron correlation has been awaited. Time-dependent density functional theory (TDDFT) is widely used for excited-state calculations of various molecules. Including the electron correlation through the exchange–correlation functional, TDDFT is known to give highly accurate results in spite of the simplicity and the low-computational cost. In this work, we have implemented the analytical TDDFT gradient method in the NTChem programs. Our implementation is based on the compact fully variational derivation of the geometrical derivatives presented by Furche and Ahlrichs. Required higher-order functional derivatives of these exchange correlation functionals for the relaxed one-particle and two-particle density matrices have been derived and implemented into efficient computer codes with the aid of a newly-developed computerized symbolic algebra system. Various DFT functionals including the recently proposed range-separated hybrid functionals and meta–generalized gradient approximation (meta-GGA) functionals are applicable to the analytic energy gradient calculations for both excited singlet and triplet excited states of a closed shell molecule and for multiplet states of an open-shell molecule. In the next financial year, we will develop transition properties and nonadiabatic coupling constant matrix elements, which is the key quantity in the description of excited-state dynamics.

8.3.4. Development of relativistic quantum Monte Carlo method

We have developed a relativistic quantum Monte Carlo (QMC) method for the accurate evaluation of the electronic state of molecular systems including both electron correlations and relativistic effects. The developed method has been implemented in a program code for a massively parallel environment. The QMC method has advantage over post Hartree–Fock methods in memory requirement, scaling of computational cost, and parallelization. This is because the MC integration can be easily parallelized and has less limitation on the integrand and a compact form of wave function is available in the QMC calculation. To extend the relativistic variational Monte Carlo method, the extension to more precise diffusion Monte Carlo (DMC) method and the inclusion of spin-orbit interaction were investigated. We have developed a relativistic DMC method based on the spin-free formalism of the zeroth order regular approximation (ZORA) Hamiltonian. The Green's function is derived from the ZORA Hamiltonian and approximated in the short-time expression in the developed method. The developed ZORA-DMC method can simultaneously evaluate both electron correlations and scalar relativistic effects and its computational cost is comparable to the nonrelativistic DMC method. This research has been accepted as the article in the Journal of Chemical Physics. The spin-orbit interaction has important effects on several molecular properties e.g. spectra of transition metal systems. Following the nonrelativistic two-component extension by Ambrosetti et al., we have developed the two-component ZORA method. The developed method is implemented in the QMC program for the use in connection with spin–orbit self-consistent field (SCF) program of the NTChem program package. In order to reduce high computational cost of the QMC, a hierarchic sparse algebra library for matrices with moderate sparseness is under development. The tuning of the serial code and the development of its parallel version is now going on.

8.3.5. Development of all-electron two-component relativistic crystal orbital theory

Relativistic effects such as spin-orbit effects often take very important roles for structural and thermochemical properties of nano-materials containing heavy elements. The robust theories and methodologies have been desired for the elucidation and reliable prediction of relativistic effects in nano-materials from theoretical and computational approach. We have developed a all-electron two-component relativistic theory for periodic systems in the framework of crystal orbital theory to treat the relativistic effects in nano-materials. The theory is based on the third-order Douglas–Kroll approximation including the spin–orbit effects and the crystal orbital theory employing the periodic boundary conditions and the localized basis functions. The use of localized basis functions correctly reproduces the electronic state of atomic inner shells where the relativistic effects are significant. In our theory, Gaussian basis functions are employed for localized basis functions. The use of Gaussian basis functions makes the calculations of molecular integral easy. We also developed a spin–orbit

self-consistent field scheme employing localized Gaussian basis functions. With this method, the all-electron calculations including the scalar and spin–orbit relativistic effects can be performed for heavy elements in periodic systems with the reasonable computational costs and chemical accuracies.

8.3.6. Development of RI-PBC method for first-principles-based material simulation

There are many chemically and physically unclear phenomena in the solid-state catalysts, photovoltaic cell, solar battery, and battery reaction, where molecules intricately and varyingly interact with metal and semi-conductor surfaces. Many of surface phenomena are difficult to directly observe by experimental methods, but their deep understandings are strongly demanded to develop highly-functionalized materials and chemical systems, and therefore the powerful assistances of simulation technologies are expected. However, the periodic boundary conditions are theoretically required to consider surface systems, and its theoretical and computational treatments are under developing. In addition, calculations with the periodic boundary conditions require for much more CPU-costs compared with isolated molecular systems. So, we have been developing the RI-PBC method to reduce the calculation costs for material and surface simulations. In the RI-PBC method, the electron densities are described by auxiliary basis functions, similar to the ordinary theory for isolated molecules, but we needed additional considerations on suitable cutoff criteria and the neutrality of the unit cell. In the following fiscal year, we will brush up the RI-PBC method, and apply it for interesting surface systems.

8.3.7. HPC usability for quantum-chemistry program

First-principles quantum chemistry methods are expected to apply for various scientific and engineering fields over pure chemical areas. In order to respond to such expectations, the usability for quantum-chemistry program is required for, but it is gradually becoming difficult to develop the hilly parallelized programs with complex quantum-chemistry theories. Therefore, we study to embed a interpreter computer language into our quantum chemistry program, because interpreter languages usually have a rich description capability compared with compiler computer language such as C/C++ and Fortran. In this study, we examined the Perl, Tcl, Ruby, and Python interpreter language, and concluded that Python can be easily embedded into our quantum chemistry program without sacrificing the computational speed. Actually, we implemented the DIIS-SCF loop by Python, and the program with embedded Python can execute first-principles quantum chemistry calculations in the same computational time, compared with the pure C++ and Fortran program. We also confirmed that our Python embedding technique can be applicable for "K" computer. In the next fiscal year, we will develop and sophisticate the RI-PBC method by using this embedded Python technology.

8.3.8. Theoretical investigation of novel chemical reaction within supramolecular assembly

Supramolecular assembly has recently attracted attention because of its novel functions such as stabilization of reactive species, molecular recognition, and catalytic activity. The Raymond group reported that chiral supramolecular assembly [Ga4L6]-12 (Fig.) encapsulate a cationic substrate and show the high catalytic activity for the aza-Cope rearrangement of substrate. They also show that enantiopure (Δ or Λ structure) [Ga4L6]-12 promote the aza-Cope rearrangement enantioselectivity. While many experimental studies have been performed, the detailed mechanism of the catalytic activity and enantioselectivity are not clear. We investigated the catalytic activity and enantioselectivity of supramolecular assembly [Ga4L6]-12 by means of ab initio MO calculation. To clarify the origin of enantioselectivity, we compare two minimum energy pathways (MEPs) of aza-Cope rearrangement in which R and S structure are produced within an assembly. Differences in the stability of reactant structure, reaction barrier and length of MEP indicate that R structure is favorably produced within a Δ structure [Ga4L6]-12. We also examine the catalytic activity for aza-Cope rearrangement by comparing reaction pathway with and without assembly. Since the reaction barrier is almost same each other, it is indicated that the enthalpic contribution is dominant for rate acceleration.
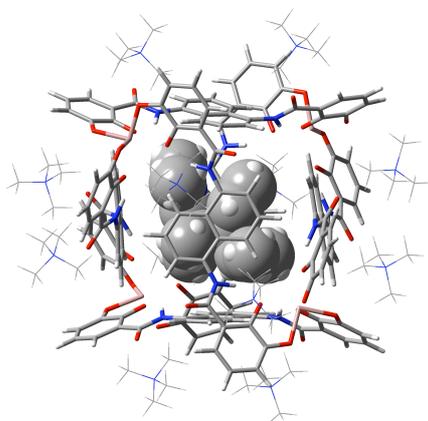
Fig. Ga4L6(L=bis(2,3-dihydroxybenzamido)naphthalen

8.3.9. New scheme to compute pKa value of amino acid

Toward the material science, the design of reaction is the most important part. Protein and its analog model complex show interesting properties and depend on the surroundings. As an example for environment dependency, each enzyme has an its optimal pH as well as optimal temperature. The pKa value is one of the criteria for the protonation of amino acid. pKa plays a key role even in chemistry, And to compute pKa is necessary for the development of the field. Nevertheless, it is surprising that no quantum chemical approach has been done for its system because of the technical difficulty such as the estimation for the energy of proton or computational costs. We here proposed a

new method to compute the pKa value on the basis of the concept for a calibration curve method. We show one of our results for pKa values of serines in Tryptophan cage (Trp-cage, 300+ atoms). From the figure below, there exists a clear difference whether OH group of serine turns outside or inside of the protein. With some assumptions, we derived the pKa values of tyrosines and serines in chignolin and a tryptophan cage. We obtained quite different pKa values of adjacent serines in the tryptophan cage; the pKa value of the OH group of Ser13 exposed to bulk water is 14.69, whereas that of Ser14 not exposed to bulk water is 22.45 because of the internal hydrogen bonds.
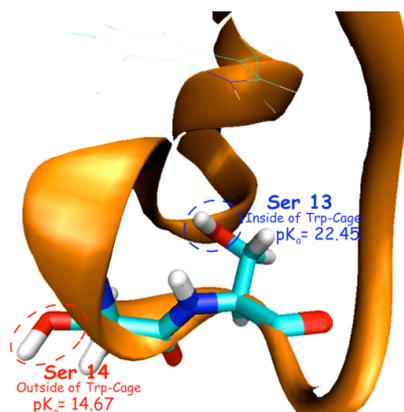
8.4. Schedule and Future Plan

In the next financial year, we will release the first version of the NTChem program suite on the K computer. We intend to continue adopting users' requests and to improve NTChem after its release, with the aim of making it more convenient and usable for researchers in many fields. We expect that NTChem will enable, for example, researchers to predict the structures of biological molecules as they relate to drug actions, and to elucidate the mechanisms by which nano-materials exhibit their unique functions.

8.5. Publication, Presentation and Deliverables

(1)   Journal Papers

1. Y. Nakatsuka, T. Nakajima, "Relativistic diffusion Monte Carlo method: Zeroth-order regular approximation-diffusion Monte Carlo method in a spin-free formalism", J. Chem. Phys. 137, 154103 (2012).

2. T. Yoshizawa, T. Nakajima, "A new computational scheme for the spin-orbit part of zero-field splitting tensor", Chem. Phys. Lett. 549, 108–112 (2012).

(2)   Conference Papers

1. M. Katouda, T. Nakajima, S. Nagase, "Development of efficient computational techniques and codes for second-order Møller–Plesset perturbation calculation of extended systems",

Proceedings of JSST 2012, 338–343 (2012).

2. T. Nakajima et. al, Chapter 1 in "Computational chemistry for large molecules", Kagaku dojin (2012). (in Japanese)

(3) Invited Talks

1. M. Katouda, "Development of computational techniques for highly accurate quantum chemical calculations on multicore massively parallel cluster systems", Annual Meeting of Japan Society for Industrial and Applied Mathematics-Young Researchers Group, Tokyo, 26 Dec. 2012. (in Japanese)

2. T. Shimazaki "Ab-initio band structure calculation with screened Hartree-Fock (HF) exchange potential", Cambodian Malaysian Chemical Conference, Siem Reap, 19 Oct. 2012.

3. T. Shimazaki "Effects of screened Hartree-Fock (HF) exchange term on first-principle band structure calculations with periodic boundary conditions", 17th Malaysian Chemical Congress, KUALAL LUMPUR, 15 Oct. 2012.

4. T. Nakajima, "Relativistic effects on quantum chemistry (1)", CMSI summer school, Yamagata, 21 Aug. 2012. (in Japanese)

5. T. Nakajima, "Relativistic effects on quantum chemistry (2)", CMSI summer school, Yamagata, 22 Aug. 2012. (in Japanese)

6. Y. Akinaga, T. Nakajima, "Development of two-component relativistic coupled-cluster methods for molecular ground- and excited states", CJK-WTCC-2012, Beijing, 22 Jul. 2012.

7. M. Katouda, T. Nakajima, "Efficient quantum chemical calculations of macromolecules", CJK-WTCC-2012, Beijing, 20 Jul. 2012.

8. M. Katouda, "Massively parallel quantum chemical calculations with K computer", RIKEN Yokohama Institute Seminar, Yokohama, 2 Jul. 2012.

9. T. Nakajima, "Theoretical molecular science and K computer", The surface science society of Japan, Kobe, 6 Apr. 2012.

(4) Posters and presentations

1. M. Katouda, T. Nakajima, "Massively parallel second-order Møller–Plesset perturbation calculations on K computer", 3rd AICS International Symposium, Kobe, 28 Feb. 2013. (Poster)

2. Y. Nakatsuka, T. Nakajima, "Development of spin-orbit ZORA quantum Monte Carlo method for atoms and molecules", 3rd AICS International Symposium, Kobe, 28 Feb. 2013. (Poster)

3. Y. Akinaga, T. Nakajima, "Two-component relativistic general-order coupled-cluster methods for excitation energy and ionization potential", 3rd AICS International Symposium,

Kobe, 28 Feb. 2013. (Poster)

4. T. Shimazaki, T. Nakajima, "Development of first-priniciples quantum chemistry program with embedded Python interpreter", 2nd AICS International Symposium, Kobe, 28 Feb. 2012. (Poster)

5. Y. Ootani, Y. Akinaga, T. Nakajima, "Theoretical exploring of reaction pathway of aza-Cope rearrangement in supramolecular assembly", 3rd AICS International Symposium, Kobe, 28 Feb. 2013. (Poster)

6. M. Katouda, T. Nakajima, S. Nagase, "Development of efficient computational techniques and codes for second-order Møller–Plesset perturbation calculation of extended systems", JSST2012, Kobe, 27 Sep. 2012.

7. M. Kamiya, H. Sekino, T. Nakajima, "Nonlinear optical property calculations by the time-dependent density-functional method", 6th Annual Meeting of Japan Society for Molecular Science, Tokyo, Japan, 18 Sep.–21 Sep. 2012. (Poster in Japanese)

8. M. Katouda, T. Nakajima, "MPI/Open-MP hybrid parallel RI-MP2 algorithm for massively parallel calculations of large molecules", Annual Meeting of Japan Society for Molecular Science 2012, Tokyo, 21 Sep. 2012. (in Japanese)

9. Y. Ootani, Y. Akinaga, T. Nakajima, "Theoretical exploring of reaction pathway of aza-Cope rearrangement in supramolecular assembly", Annual Meeting of Japan Society for Molecular Science 2012, Tokyo, 19 Sep. 2012. (in Japanese)

10. Y. Akinaga, T. Nakajima, "Development of two-component relativistic coupled-cluster methods: application to molecular ground and excited states", 6th Annual Meeting of Japan Society for Molecular Science, Tokyo, Japan, 18 Sep. 2012.

11. Y. Nakatsuka, T. Nakajima, "Relativistic QMC approach with spin-orbit interaction", Annual Meeting of Japan Society for Molecular Science, Tokyo, 18 Sep. 2012. (in Japanese)

12. M. Katouda, T. Nakajima, "Development of two-component relativistic crystal orbital theory", 15th Annual Meeting of Theoretical Chemistry Society in Japan, Sendai, 24 May 2012. (Poster in Japanese)

(5) Patents and Deliverables
     -None

9. Computational Materials Science Research Team

9.1. Team members

Seiji Yunoki (Team Leader)

Yuichi Otsuka (Research Scientist)

Shigetoshi Sota (Research Scientist)

Atsushi Yamamoto (Postdoctoral Researcher)

Sandro Sorella (Senior Visiting Researcher)

Machiko Matsusue (Assistant)

9.2. Research Activities

Understanding the properties of strongly correlated quantum systems and developing efficient numerical tools to simulate these systems are, since many years, one of the central problems in modern condensed matter physics. Phenomena such as high-T_c superconductivity, geometrically frustrate quantum systems, heavy electrons, and spin liquid phases still remain elusive to a complete understanding. Comprehension of strongly correlated quantum systems is believed to be also very important for chemistry in controlling chemical reactions and for biology in designing multi functional proteins. Methods we employ to tackle these quantum many-body problems share common features also with those used in elementary particle physics. We thus believe that our project is important to lead to a significant advancement of knowledge in one of the most active fronts of research. It will further have an impact on several different disciplines in basic and applied sciences.

The computational materials science research team conducts researches on searching a novel quantum state of matter emerging in the strongly correlated quantum systems and designing new functional materials by large scale simulations. Such new phenomena and functionalities very often arise due to the strong correlations, where the approximations based on one-particle picture such as the mean-filed treatment breakdown and analytical approaches are less abundant. Furthermore, understanding various competing orders and the nature of phased transitions observed in real materials requires going beyond small systems. The tremendous amount of effort has been devoted to develop new simulation methods and test their ability and validity for large-scale simulations.

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

1) We develop a large scale quantum Monte Carlo (QMC) simulation method, which is one of the most reliable and efficient techniques for Hubbard-type lattice models. Typical target systems we aim are of the order of 10,000 electrons on lattice systems for which the notorious minus sign problem does not occur.

2) We develop a density matrix renormalization group method (DMRG) for two dimensional

quantum systems such as the Hubbard model on the triangular lattice and geometrically frustrated spin-1/2 Heisenberg models. We have been developing massively parallel DMRG algorithms to perform large-scale calculations on the K computer with high performance. Our DMRG can calculate not only ground state static properties but also dynamical quantities at finite temperatures as well as properties for systems which are out of equilibrium.

9.3. Research Results and Achievements

9.3.1. QMC simulations for Hubbard model on honeycomb lattice

We have developed the auxiliary filed quantum Monte Carlo method for lattice fermion systems at zero temperature. Since numerical calculations involved in this scheme are mostly linear algebraic procedure such as matrix-matrix product and numerical orthogonalization, we can take advantage of the highly optimized numerical library on the K computer to calculate physical observables with a high degree of accuracy on quite large systems. We have applied this improved code to the half-filled Hubbard model on the honeycomb lattice, in which a gapped spin-liquid phase have been predicted to appear by a German group [Z. Y. Meng *et al*., Nature **464**, 847 (2010)]. Since geometrical frustration, being absent in the honeycomb lattice, is supposed to be a key ingredient for the stable spin-liquid phase, this issue has been a major topic of debate. Our numerical results performed on the lattice sizes up to *N*=2,596, about 4 times larger than the German group, have clearly found that this spin-liquid phase is quite unlikely, confirming a conventional scenario of the Mott transition from semi-metal to antiferromagnetic Mott insulating state (see Fig.1).
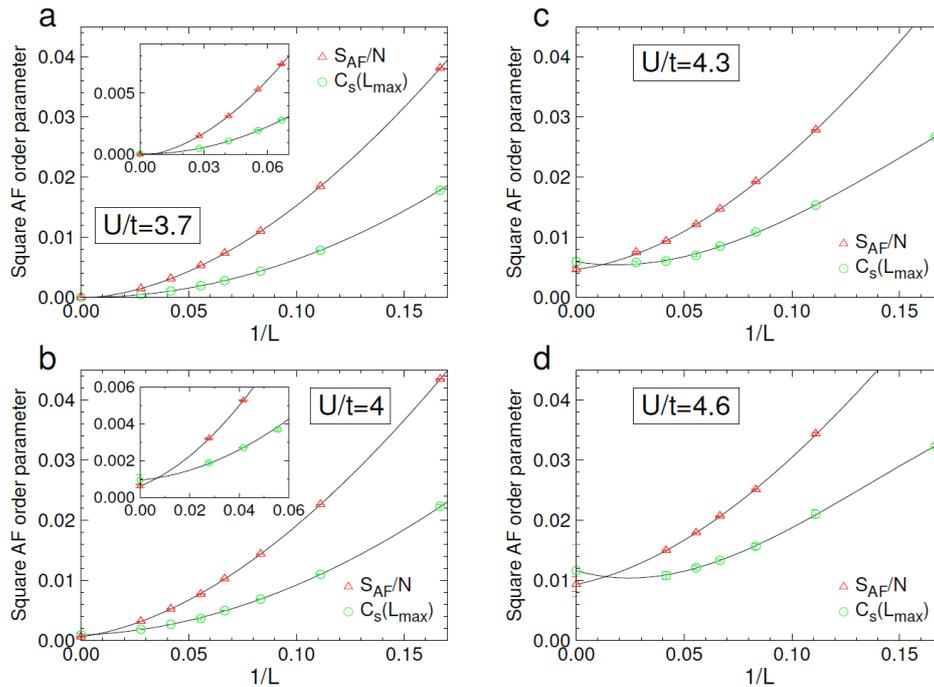
Fig. 1: Finite size scaling of spin-spin correlations functions for the Hubbard model on the honeycomb lattice at half-filling. Spin structure factor S_{AF} and spin-spin correlations at the maximum distance $C_s(L_{max})$ are denoted by triangles and circles, respectively. Here L is the linear size of clusters containing $N=2L^2$ sites. Antiferromagnetic order parameter m_s^2 is estimated by finite size extrapolating S_{AF} and $C_s(L_{max})$ to L infinite. U/t used is indicated in the figures. [taken from S. Sorella, Y. Otsuka, and S. Yunoki, Scientific Reports, **2**, 992 (2012)]

9.3.2. Development of massively parallel DMRG algorithm

The DMRG method can be used to investigate properties on low-dimensional strongly correlated quantum systems. Especially, it is well known that the DMRG method is very suitable for studying one-dimensional strongly correlated quantum systems since the number m of truncated states which should kept for the accurate DMRG calculations is moderate (~several hundreds). However, keeping the large number m of states, we can in principle employ the DMRG method to study two-dimensional strongly correlated quantum systems, which of course requires the huge computational cost for the memory usage and computational time since the dimension of the Hamiltonian is proportional to m^2.

Fig. 2: The parallelization of the matrix-matrix product, which appears in the DMRG algorithm. For the Hamiltonian (left matrix), we employ two MPI communicators for the column direction and the row direction. In addition, we employ a communicator for the row direction of the right matrix, which was a vector before transforming from the matrix-vector product to the matrix-matrix product.

The largest computational cost in the DMRG procedure is the matrix-vector product in the eigenvalue problem of the Hamiltonian. Thus, the efficient execution of the matrix-vector product is the key ingredient to successfully develop an effective algorithm of the massively parallel DMRG method. In the DMRG procedure, we consider not only a system but also an environment. Namely, we can decompose the Hamiltonian treated in the DMRG procedure into the system and the environment. With this transformation, the Hamiltonian, which is m^2 dimension, is given by the

system and the environment, which is given by *m* dimension Hamiltonian. As the result of this transformation, the matrix-vector product becomes the matrix-matrix product. For this matrix-matrix product, we define three MPI communicators for the column and row directions of the Hamiltonian and the row direction of the matrix, which was a vector before the transformation (see Fig. 2). Using this parallelization scheme for the matrix-matrix product, the communications are localized within the small number of MPI processes. In Fig. 3, we show the parallelization effect and the computational efficiency on 12,288 nodes and 24,576 nodes for strong scaling. As seen in Fig.3, the parallelization efficiency is almost 90% between 12,288 nodes and 24,676 nodes on the K computer. We can also see in Fig.3 that we achieve ~1.73 PFlops, which is 54.9% of the theoretical maximum performance achieved on 24,576 nodes on the K-computer.
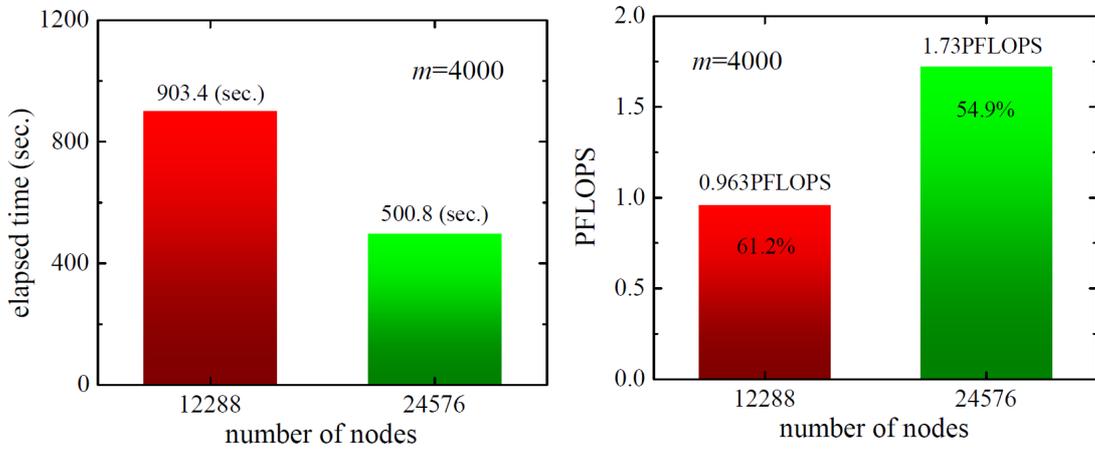
Fig. 3: The elapsed time (left) and the computational effeciency (right) using 12288 nodes and 24576 nodes on the K-computer. This benchmark is performed by the dynamical DMRG calculations on the one-dimensional extended Hubbard model using *m*=4000.

We should also emphasize that our massively parallel DMRG algorithm can be readily extended to the dynamical DMRG method, finite temperature DMRG method, and time-dependent DMRG method with almost the same performance.

9.3.3. Development of two-dimensional DMRG algorithm for K-computer

We have developed a massively parallel two-dimensional DMRG algorithm to study two-dimensional strongly correlated quantum systems. The two-dimensional DMRG algorithm is based on our massively parallel DMRG algorithm for one-dimension systems described in 3.2 (see also Fig. 2). Introducing the long-range interactions into the "one-dimensional" DMRG algorithm, we can develop a massively parallel two-dimensional DMRG. The long-range interactions are given to construct two-dimensional lattice systems. Since the numerical calculations for these long-range

interactions can be performed separately, the two-dimensional DMRG algorithm is suitable for massively parallel computations. Our developed two-dimensional DMRG shows high performance, similar to the one developed for the massively parallel one-dimensional DMRG. We expect to be able to perform the largest two-dimensional DMRG calculations ever in this research field of strongly correlated quantum systems, and currently we have been working on the Hubbard model on the triangular lattice and geometrically frustrated spin 1/2 Heisenberg models in two dimensions.

9.3.4. Dynamical DMRG study of optical conductivity

Using our developed dynamical DMRG, we have studied the optical responses of one-dimensional strongly correlated electron systems. In this academic year, we have focused on the nonlinear optical response of one-dimensional Mott insulators such as Sr_2CuO_3. The Sr_2CuO_3 is known as a typical one-dimensional Mott insulator. The Sr_2CuO_3 is expected to develop a new optical switching device without an electrical signal, since the giant nonlinear optical response and the ultra-fast relaxation process have been experimentally observed. In the present study, we have investigated the giant nonlinear optical response by using the dynamical DMRG method. We have employed a Hubbard-Holstein model, which includes a Holstein-type electron-phonon interaction to describe the one-dimensional electron system Sr_2CuO_3, since the strong electron-phonon interaction is believed to be important to understand the optical response of this system. The strong electron-phonon interaction implies that we have to keep large number of phonons, making the DMRG calculations very difficult. In addition, in order to investigate the nonlinear optical response by the dynamical DMRG method, we have to take many excitation processes into account. Therefore, we have used the K-computer and our developed massively parallel dynamical DMRG. Setting the model parameters for Sr_2CuO_3 estimated by our previous study, we have found that the nonlinear optical response shows a clearly phonon assisted spin excitation. Our result has demonstrated the importance of the electron-phonon interaction to understand the nonlinear optical response of the one-dimensional Mott insulator Sr_2CuO_3.

Using the dynamical DMRG method, we have also studied a temperature dependence of the high energy optical conductivity on a parent compound of high-*T*c cuprates. Using the finite temperature algorithm, we have calculated the optical conductivity for different temperatures. We have found that although the temperature change is small within 0 K and ~300 K, the optical conductivity is strongly redistributed in a wide range of energy up to 10~20 eV. We believe that this is one of the manifestations of the strongly correlated effects in strongly correlated materials.

9.4. Schedule and Future Plan

9.4.1. QMC simulations for even larger systems

The QMC methods in general require less memory. Therefore, we have been able to simulate 2,596 electrons by our present code, which is implemented so that one Slater determinant describing the ground-state at a fixed configuration of the auxiliary filed is stored in a single node. However, to achieve further performance needed for simulations of the order of 10,000 electrons, we have to distribute the Slater determinant into several nodes because of the capacity of memory available in the single node of the K computer. We need larger scale simulation because the direct comparison between a theoretical calculation and an experimental observation would be possible only with the simulations of this scale. The research along this line is now in progress.

9.4.2. DMRG simulations for two-dimensional systems at finite temperatures

In order to achieve high efficiency in MPI parallelization for the two-dimensional DMRG algorithm, we will adapt new algorithms to speed up the sweeping process, which is the main part of the DMRG method. In addition, we will develop the finite temperature two-dimensional DMRG method, the time dependence two-dimensional DMRG method, and the dynamical two-dimensional DMRG method. Using these newly developed massively parallel two-dimensional DMRG applications, we will study two-dimensional strongly correlated quantum systems such as spin/charge frustrated quantum systems, cold atoms in optical lattices, and strongly correlated electrons models.

9.5. Publication, Presentation and Deliverables

(1)   Journal Papers

1.   "Absence of a spin liquid phase in the Hubbard model on the honeycomb lattice", S. Sorella, Y. Otsuka, and S. Yunoki, Scientific Reports, **2**, 992 (2012).

2.   "Enhanced charge order in a photoexcited one-dimensional strongly correlated system", H. Lu, S. Sota, H. Matsueda, J. Bonca, T. Tohyama, Phys. Rev. Lett. **109**, 197401 (2012).

3.   "Monte Carlo study of an unconventional superconducting phase in Iridium oxides J_{eff}=1/2 Mott insulators induced by carrier doping", H. Watanabe, T. Shirakawa, and S. Yunoki, Phys. Rev. Lett. **110**, 027002 (2013).

4.   "Magnetic and orbital order in $(RMnO_3)_n/(AMnO_3)_{2n}$ superlattices studied via a double-exchange model with strain", S. Dong, Q. Zhang, S. Yunoki, J.-M. Liu, and E. Dagotto, Phys. Rev. B **86**, 205121 (2012).

5.   "Strain-engineered magnetic order in $(LaMnO_3)_n/(SrMnO_3)_{2n}$ superlattices", Q. Zhang, S. Dong, B. Wang, and S. Yunoki, Phys. Rev. B **86**, 094403 (2012).

6. "Kernel polynomial method on GPU", S. Zhang, S. Yamagiwa, M. Okumura, and S. Yunoki, Int. J. Parallel Prog. **41**, 59 (2013).

(2) Conference Papers

1. "Variational Monte Carlo study for superconductivity in multi-orbital systems", H. Watanabe, T. Shirakawa, and S. Yunoki, J. Phys.: Conf. Ser. **400**, 022134 (2012).

2. "d^0 ferromagnetic surface in HfO_2", G. Chen, Q. Zhang, X. Gong, and S. Yunoki, J. Phys.: Conf. Ser. **400**, 032008 (2012).

3. "Theoretical study of $J_{eff} = 1/2$ Mott insulator in Ir oxides: a strong spin-orbit coupling vs local electron correlations", T. Shirakawa, H. Watanabe, and S. Yunoki, J. Phys.: Conf. Ser. **400**, 032088 (2012).

4. "A first-principles study for electronic and magnetic properties of $LaFeO_3/LaCrO_3$ superlattices", Q. Zhang and S. Yunoki, J. Phys.: Conf. Ser. **400**, 032126 (2012).

(3) Invited Talks

1. "Recent advances in the numerical simulation of the Hubbard model", S. Sorella, S. Yunoki, and Y. Otsuka, Correlations and coherence in quantum systems, October 2012 (Évora, Portugal).

2. "Microscopic study of spin-orbit-induced Mott insulator and unconventional superconductivity in Ir oxides", S. Yunoki, IGER International Symposium on Science of Molecular Assembly and Biomolecular Systems 2012, September 2012 (Nagoya, Japan).

3. "Microscopic study of spin-orbit-induced Mott insulator and unconventional superconductivity in Ir oxides", S. Yunoki, Tsinghua-RIKEN Joint Workshop, October 2012 (Beijing, China).

4. "Defect induced ferromagnetism for a wide band gap insulator without magnetic ions", S. Yunoki, 22nd Computational Materials Design Workshop, March 2013 (Kobe, Japan).

(4) Posters and presentations

1. "Optical response on low-dimensional strongly correlated systems", S. Sota, CMSI summer school, August 2012 (Yamagata, Japan).

2. "High-energy optical response on high-Tc cuprates", S. Sota, T. shirakawa, and S. Yunoki, The Physical Society of Japan (JSP), Autumn meeting, September 2012, (Yokohama, Japan).

3. "Phase diagram of 1D fermionic optical lattices with spatially alternating interaction", A. Yamamoto and S. Yunoki, ICAP 2012: 23rd International Conference on Atomic Physics, July 2012 (Paris, France).

4. "A novel superconductivity in Ir oxides with a large spin-orbit coupling", H. Watanabe, T.

Shirakawa, and S. Yunoki, 19th International Conference on Magnetism (ICM 2012), BEXCO, Busan, July 2012 (Busan, Korea).

5. "Effective exchange interactions in 5d transition metal oxides", T. Shirakawa, H. Watanabe, and S. Yunoki, 19th International Conference on Magnetism (ICM 2012), BEXCO, Busan, July 2012 (Busan, Korea).

6. "Dynamical density matrix renormalization group study of high-energy optical conductivity in high-Tc copper-oxides", S. Sota, T. Shirakawa, and S. Yunoki, Conference on Computational Physics 2012, October 2012 (Kobe, Japan).

7. "Theoretical study of novel insulating and superconducting states in Ir oxides with large spin-orbit oupling", H. Watanabe, T. Shirakawa, and S. Yunoki, Conference on Computational Physics 2012, October 2012 (Kobe, Japan).

8. "Theoretical studies of a three-band Hubbard model with a strong spin-orbit coupling for 5d transition metal oxides Sr_2IrO_4", T. Shirakawa, H. Watanabe, and S. Yunoki, Conference on Computational Physics 2012, October 2012 (Kobe, Japan).

9. "Superfluidity of One-dimensional Trapped Fermionic Optical Lattices with Spatially Alternating Interactions", A. Yamamoto and S. Yunoki, Conference on Computational Physics 2012, October 2012 (Kobe, Japan).

10. "A Study of Parallelizing O(N) Green-Function-Based Monte Carlo Method for Many Fermions Coupled with Classical Degrees of Freedom", S. Zhang, S. Yamagiwa, and S. Yunoki, Conference on Computational Physics 2012, October 2012 (Kobe, Japan).

11. "Photoinduced spin-order destructions in one-dimensional extended Hubbard mode", H. Lu, S.Sota, H. Matsueda, J. Bonca, and T. Tohyama, "Photoinduced spin-order destructions in one-dimensional extended Hubbard mode", Conference on Computational Physics 2012, October 2012 (Kobe, Japan).

12. "Dynamical DMRG Study of Spin Excitations in Disordered Spin-Peierls Systems", K. Shinjo, S. Sota, and T. Tohyama, Conference on Computational Physics 2012, October 2012 (Kobe, Japan).

13. "Quantum Monte Carlo study of the half- filled Hubbard model on the honeycomb lattice", Y. Otsuka, S. Yunoki, and S. Sorella, Conference on Computational Physics 2012, October 2012 (Kobe, Japan).

14. "GPU-based Parallelization of Kernel Polynomial Method for Solving LDOS", S. Zhang, S. Yamagiwa, and S. Yunoki, Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems, December 2012 (Salt Lake City, USA).

15. "Dynamical DMRG study of nonlinear optical response of one-dimensional Mott insulator", S. Sota and T. Tohyama, 3rd CMSI symposium, December 2012, (Okazaki, Japan).

16. "Dynamical density matrix renormalization group study of high-energy optical conductivity

in high-Tc copper-oxides", S. Sota, T. Shirakawa, and S. Yunoki, DMRG winter school, December 2012 (Taipei, Taiwan).

17. "Massively parallel two-dimensional density matrix renormalization group method algorithm for two-dimensional strongly correlated systems", S. Sota, T. Tohyama, and S. Yunoki, QS2C International forum: International Symposium on "Strongly Correlated Quantum Science", January 2013 (Tokyo, Japan).

18. "Mott transition in the half-filled Hubbard model on the honeycomb lattice", Y. Otsuka, S. Yunoki, and S. Sorella, QS2C International forum: International Symposium on "Strongly Correlated Quantum Science", January 2013 (Tokyo, Japan).

19. "Two-dimensional density matrix renormalization method on K-computer", S. Sota, S. Yunoki, and T. Tohyama, 3rd AICS International symposium, March 2013 (Kobe, Japan).

20. "Dynamical density matrix renormalization group study of non-linear optical response of one-dimensional strongly correlated electron system", S. Sota, S. Yunoki, and T. Tohyama, APS march meeting 2013, March 2013 (Baltimore, USA).

21. "Finite temperature dynamical density matrix renormalization group study of high-energy optical conductivity in high-Tc cuprates", S. Sota, T. Shirakawa, and S. Yunoki, APS march meeting 2013, March 2013 (Baltimore, USA).

22. "Enhanced charge order in a photoexcited one-dimensional strongly correlated system", H. Lu, S. Sota, H. Matsueda, J. Bonca, and T. Tohyama, APS march meeting 2013, March 2013 (Baltimore, USA).

23. "The low-energy magnetic excitations of a three-band Hubbard model with a strong spin-orbit coupling for 5d transition metal oxides Sr_2IrO_4", T. Shirakawa, H. Watanabe, and S. Yunoki, APS march meeting 2013, March 2013 (Baltimore, USA).

24. "Theoretical study of novel superconductivity in Ir oxides with large spin-orbit coupling", H. Watanabe, T. Shirakawa, and S. Yunoki, APS march meeting 2013, March 2013 (Baltimore, USA).

25. "Dynamical DMRG study of nonlinear optical response of one-dimensional Mott insulator", S. Sota, S. Yunoki, and T. Tohyama, The Physical Society of Japan (JSP) meeting, March 2013, (Hiroshima, Japan).

26. "Dynamical DMRG Study of Spin Excitations in Disordered Spin-Peierls Systems", K. Shinjo, S. Sota, and T. Tohyama, The Physical Society of Japan (JSP) meeting, March 2013, (Hiroshima, Japan).

(5) Patents and Deliverables
   -None

10. Computational Biophysics Research Team

10.1. Team members

Yuji Sugita (Team Leader)

Jaewoon Jung (Research Scientist)

Osamu Miyashita (Research Scientist)

Ryuhei Harada (Postdoctoral Researcher)

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10.2. Research Activities

Recent advances in structural biology, atomic structures of macromolecules have been determined by X-ray crystallography and nuclear magnetic resonance (NMR). These coordinates stored in protein data bank (PDB) are utilized for academic researches or industrial usages like drug design. The 'static' atomic structures are quite useful to understand molecular mechanisms underlying protein stability, large-scale conformational changes, ligand-receptor bindings, and enzymatic reactions. However, due to the complexity and flexibility of biomolecules, dynamical information, like conformational fluctuations or transitions between different physiological states is necessary for deeper understanding of the biological phenomena.

Computer simulations based on molecular dynamics (MD) method using the macromolecular structures now become important research tools also in life sciences. Conventional MD software allows us to carry out simulations of proteins or nucleic acids for several hundred nsec or longer. We aim to develop new MD software (GENESIS), which is highly parallelized for the usage of K computer. GENESIS also contains enhanced conformational sampling methods and multi-scale and multi-resolution simulation methods. Using GENESIS, we would like to start cellular-scale simulations based on the molecular representation of proteins and other biomolecules.

10.3. Research Results and Achievements

10.3.1. Parallelization of molecular dynamics simulation codes

GENESIS consists of two molecular dynamics simulation programs, named as ATDYN and SPDYN. In ATDYN, force decomposition is implemented as a parallel scheme, whereas SPDYN employs spatial decomposition scheme for obtaining a good scalability in massively parallel supercomputers. By last year, we have almost finished the development and parallelization of ATDYN and in this year, we focused on the development of SPYN. In SPDYN, we use a modified midpoint method originally developed by D.E.Shaw and his colleagues. In the original midpoint method, two particles interact on a particular box if and only if the midpoint of the segment connecting them falls within the region of space associated with that box. This method reduces the amount of communications between different processors during the nonbonded interaction calculations. We employ smooth particle mesh ewald method for long-range electrostatic interactions. In the reciprocal part of electrostatic calculations, we use three-dimensional decomposition of fast Fourier transform (FFT). Due to these schemes, we could get a good scalability in MD simulations.

10.3.2. Enhanced conformational sampling techniques

Free-energy landscapes of proteins or other biomolecules have usually rugged free-energy landscapes with huge number of local energy minima. Due to the complexity, the conventional MD has limitation in surveying all of the possible conformations. One of the possible ways to overcome this is to pre-define collective variables and bias the dynamics by adding the history-dependent potential (meta-dynamics). Recently, we have introduced well-tempered meta-dynamics scheme in ATDYN where new Gaussian is added at fixed time interval as a history-dependent bias potential. In addition to this scheme, three addition meta-dynamics schemes are being developed in ATDYN: multiply-walker, parallel-tempered, and bias-exchange meta-dynamics.

10.3.3. Protein stability under cellular environments

The effect of cellular crowding environments on protein structure and stability is a key issue in molecular and cellular biology. The classical view of crowding emphasizes the volume exclusion effect that generally favors compact, native states. Here, results from molecular dynamics simulations and NMR experiments show that protein crowders may destabilize native states via protein-protein interactions. In the model system considered here, mixtures of villin head piece and protein G at high concentrations, villin structures become increasingly destabilized upon increasing crowder concentrations. The denatured states observed in the simulation involve partial unfolding as well as more subtle conformational shifts. The unfolded states remain overall compact and only partially overlap with unfolded ensembles at high temperature and in the presence of urea. NMR

measurements on the same systems confirm structural changes upon crowding based on changes of chemical shifts relative to dilute conditions. An analysis of protein-protein interactions and energetic aspects suggests the importance of enthalpic and solvation contributions to the crowding free energies that challenge an entropic-centered view of crowding effects.
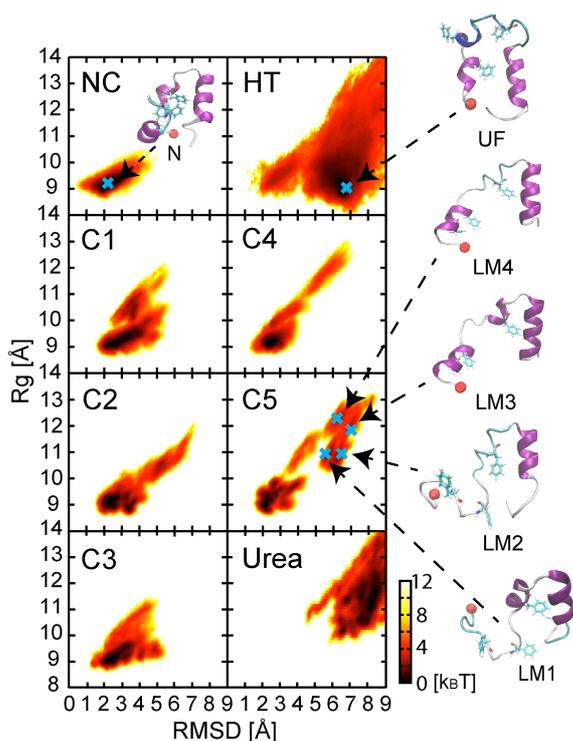
Figure 1. Potential of mean force (PMF) as a function of RMSD and Rg of villin at different protein concentrations (C1 (12%vol), C2 (17%vol), C3 (25%vol), C4 (37%vol), C5 (43%vol)) in units of k_BT.

10.3.4. Data assimilation algorithm for analyzing protein conformational motions

Protein functions, such as enzymatic catalysis and signal transduction, are mediated by the conformational transitions on the complex energy landscape in high-dimensional conformational space. The recent advances in computational power enable us to sample such conformation transitions of small proteins with all-atom molecular dynamics simulations. For moderate-sized proteins typical in living cells, however, it is still challenging to observe functionally relevant motions or conformational changes in silico. In order to simulate functionally relevant conformational transitions in moderate-sized proteins, we are developing a methodology to sample hidden conformation states or variables from low-dimensional experimental data, such as

single-molecule FRET photon trajectories. In this methodology, called the data assimilation, a bunch of (coarse-grained) protein models are concurrently simulated and also filtered (resampled) during the simulation in a bootstrapping manner according to the likelihoods with the experimental data. In this fiscal year, we have implemented the basic algorithm (particle filter) and an advanced version (merging particle filter) in GENESIS, and studied the performance of the algorithms by using a coarse-grained model (mixed elastic network model) and emulated single-molecule FRET trajectories. In the future, we are planning to apply the code to real single-molecule FRET trajectories.
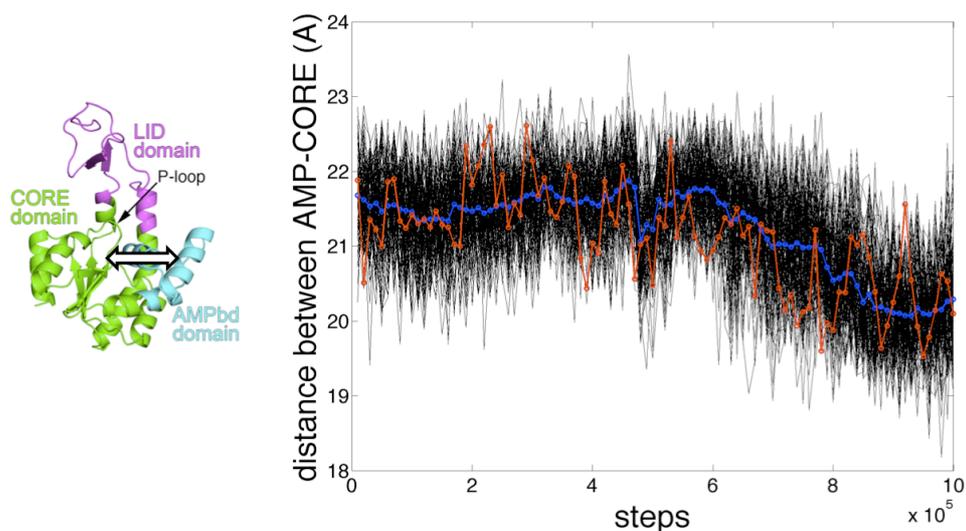
Figure 2. Estimation of a hidden variable from emulated single-molecule FRET data by using the data assimilation. The FRET data was emulated by a simulation of a coarse-grained model of Adenylate kinase. From the distance trajectory between the dyes attached to the CORE and LID domains (colored by green and magenta in the left panel, respectively), the FRET data was created. Here, we considered the distance between the CORE and AMPbd domains (colored by cyan) as the hidden variable and estimated that from the FRET data using the particle filter simulation. In the right panel, the "true" answer is indicated by the red line, and the estimation is the blue line. The distances of all particles are superimposed by the black lines.

10.4. Schedule and Future Plan

By the end of FY2013, we will open the source code of GENESIS version 1.0 for academic researchers as well as industrial users under GPL license. We need to finish the development of classical MD simulations and REMD simulations in GENESIS in FY2013. After that, we try to improve the parallel performance of GENESIS, by introducing new ideas and schemes. We also introduce new conformational sampling algorithms and coarse-grained models of biomolecules in GENESIS. We are also planning to develop QM/MM molecular dynamics module in our code in

collaboration with Dr. Nakajima's team at RIKEN AICS. By combining with parallelized QM code developed by Dr. Nakajima's group, we can perform highly parallelized QM/MM molecular dynamics simulations or QM/MM free-energy calculations of biomolecules or other molecular systems.

10.5. Publication, Presentation and Deliverables

(1) Journal Papers

1. Ryuhei Harada, Naoya Tochio, Takanori Kigawa, Yuji Sugita, and Michael Feig: "Reduced Native State Stability in Crowded Cellular Environment Due to Protein-Protein Interactions", *J. Am. Chem. Soc.* **135** (2013) 3696-3701.

2. Jaewoon Jung, Suyong Re, Yuji Sugita, and Seiichiro Ten-no: "Improved constrained optimization method for reaction-path determination in the generalized hybrid orbital quantum mechanical/molecular mechanical calculations", *J. Chem. Phys.* **138** (2013) 044106.

3. Yasuhiro Matsunaga, Ryutaro Koike, Motonori Ota, J.H. Tame, and Akinori Kidera "Influence of Structural Symmetry on Protein Dynamics", *PLoS ONE* **7**, (2012) e50011.

(2) Conference Papers
    -None

(3) Invited Talks

1. Ryuhei Harada, ○Yuji Sugita and Michael Feig: "Protein Crowding Affects Hydration Structure and Dynamics", 2012 Telluride Workshop on Protein and Peptide Interactions in Cellular Environments, Collorado, USA, June 26, 2012.

2. ○Yuji Sugita, Ryuhei Harada, and Michael Feig: "Hydration structure and dynamics under protein crowding environments", ACS meeting, Philadelphia, USA, August 21, 2012.

3. ○Yasuhiro Matsunaga "Exploring the minimum free energy path of conformation transition in Adenylate Kinase by using the finite-temperature string method", Symposium "New Frontier of Chemical Reaction Path Search 2012", Tokyo, September 21-22, 2012.

4. ○Yuji Sugita: "How macromolecular crowding affects protein stability and dynamics?", 4th Biosupercomputing Symposium, December 3, 2012.

(4) Posters and presentations

1. Jaewoon Jung, Takaharu Mori, and Yuji Sugita, "Hybrid (MPI+OPENMP) parallelization of molecular dynamics with cell-pair Verlet list", The 26h Annual Meeting of the Molecular Simulation Society of Japan, Fukuoka, November 26-28, 2012

2. Yasuhiro Matsunaga, Takaharu Mori, and Yuji Sugita, "Data Assimilation in Molecular Dynamics Simulation", The 26th Annual Meeting of the Molecular Simulation Society of Japan, Fukuoka, November 26-28, 2012.

3. Jaewoon Jung, Suyong Re, Yuji Sugita, and Seiichiro Ten-no, "Improved constrained optimization method for reaction-path determination in quantum mechanical/molecular mechanical calculations", Biophysical Society 57th Annual Meeting, Philadelphia, USA, February 2-6, 2013

4. Ryuhei Harada, Yuji Sugita, and Michael Feig, "Stability of proteins in cellular environments", Biophysical Society 57th Annual Meeting, Philadelphia, USA, February 2-6, 2013

5. Jaewoon Jung, Takaharu Mori, and Yuji Sugita, "Hybrid parallelization of Molecular dynamics with cell-pair Verlet list", The third AICS International Symposium, Kobe, February 28-March 1, 2013

6. Takaharu Mori, Jaewoon Jung, and Yuji Sugita, "Development of a New Replica-Exchange Molecular Dynamics Method for Bio-Membrane Systems", The third AICS International Symposium, Kobe, February 28-March 1, 2013

7. Yasuhiro Matsunaga, Takaharu Mori, Jaewoon Jung, and Yuji Sugita, "Tracking Protein Dynamics from Single-Molecule FRET via sequential Monte Carlo filtering", The third AICS International Symposium, Kobe,February 28-March 1, 2013

(5) Patents and Deliverables
    -None.

11. Particle Simulator Research Team

11.1. Team members

Junichiro Makino (Team Leader)

Keigo Nitadori (Research Scientist)

Masaki Iwasawa (Postdoctoral Researcher)

Yuri Iida (Assistant)

11.2. 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 refinement. 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.

11.3. 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.

11.3.1. High-performance gravitational N-body solver.

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

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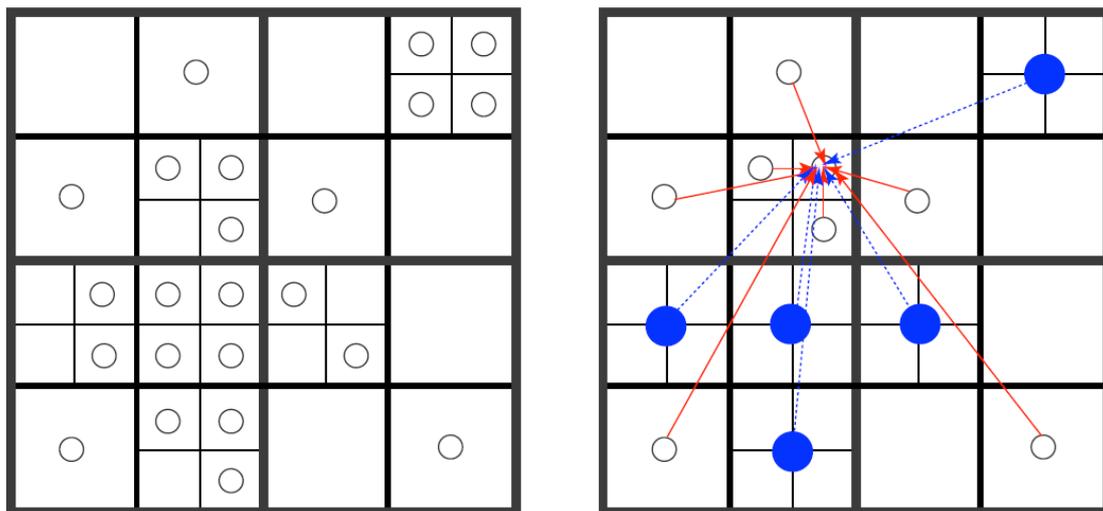
Figure 1. Basic idea of the tree algorithm

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^3M and TreePM

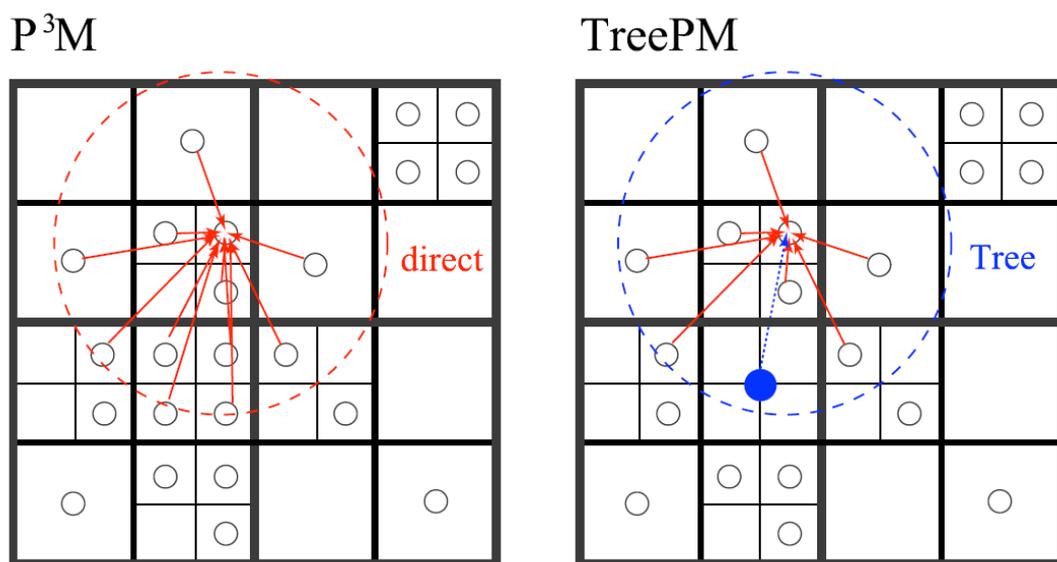In order to map the problem to the distributed-memory parallel computer such as the K computer, we adopted the approach to divide the space into domains and assign particles in one domain to one calculation node. We used the orthogonal recursive multisection method developed by the team leader some years 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.
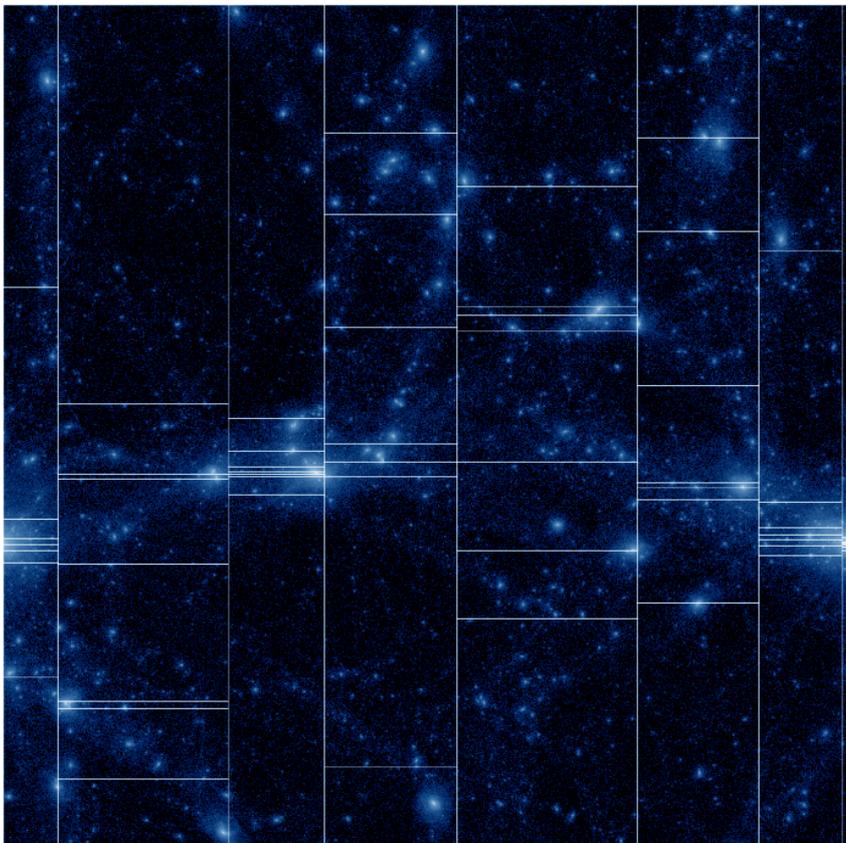

Figure 3. Recursive multisection in two dimension

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

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

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

11.3.2. Particle Simulation Platform.

Currently, we are in the design phase for the particle simulation platform. We have determined what algorithms we should use for the domain decomposition and load balance, but have not made the detailed specification yet.

11.3.3. Improvements on SPH.

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

We have been working on the possible solution on this problem, and have made two significant steps in this year. The first one is the generalization of the density-independent SPH to an arbitrary

equation of state, and the second one is its further generalization which requires the continuity of neither density nor pressure.

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

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

11.4. Schedule and Future Plan

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

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

11.5. Publication, Presentation and Deliverables
 (1)   Journal Papers
1.   Prog. Theor. Exp. Phys. (2012) 01A303 doi: 10.1093/ptep/pts029   Astrophysics with GRAPE *Junichiro Makino   and   Takayuki Saitoh
2.   10.1016/j.newast.2012.01.003 Farr, W. M., Ames, J., Hut, P., *Makino, J.,   McMillan, S., Muranushi, T., Nakamura, K., *Nitadori, K., and Portegies Zwart, S.,   "PSDF: Particle Stream Data Format for N-body simulations",   NewA,   17,   520-523(2012)

3. 10.1016/j.newast.2011.09.001 Tanikawa, A., Hut, P., and *Makino, J., "Unexpected formation modes of the first hard binary in core collapse", NewA, 17, 272-280(2012)

4. 10.1016/j.newast.2011.07.011 *Saitoh, T. R. and *Makino, J., "A natural symmetrization for the plummer potential", NewA, 17, 76-81(2012)

5. 10.1088/0004-637X/746/1/26 Matsui, H., *Saitoh, T. R., *Makino, J., Wada, K., Tomisaka, K., Kokubo, E., Daisaka, H., Okamoto, T., and Yoshida, N., "Origin of Multiple Nuclei in Ultraluminous Infrared Galaxies", ApJ, 746,

(2) Conference Papers
   -None

(3) Invited Talks

1. Junichiro Makino, Application and Architecture of Exascale Computing --- To make sure that we will not cry "This is not what I want!" ,RIRONKON Symposium 2012, "New developments of Computational Astrophysics", 2012/12/23

2. Junichiro Makino, Possibility of Galactic Paleoclimatology --- Global climate change of the Earth and the dynamics of the galactic disk, Symposium of GCOE program From The Earth To "Earths" Interdisciplinary Study On Habitable Planets, 2012/11/10

3. Junichiro Makino, From supercomputer development to science --- Lessons learned in GRAPE project. Meeting of JSPS committee No. 165 on Silicon VLSI system

4. Junichiro Makino, Exaflops and Beyond --- The view of the HPCI WG and my view Meeting on the Acceleration Technology --- Can we make computers equivalent to the human brain? 2012/9/6-7

5. Junichiro Makino, From the point of view of applications --- To make sure that we will not cry "This is not what I want!" HPC Forum, 2012/8/20

6. Junichiro Makino, Research on the future HPCI system with accelerators --- Basic concepts of the architecture 7th SDHPC workshop, 2012/7/31

7. Junichiro Makino, From the K computer to Exascale --- Development of supercomputers andthe role of National projects. Software Symposium SS2012, 2012/6/14

(4) Posters and presentations

1. Keigo Nitadori, "SIMD Class Library for HPC-ACE Instructions and its Application for N-body Kernel", The 3rd AICS international Symposium, 28 Feb – 1 Mar 2013

2. Masaki Iwasawa, "Particle-Particle Particle-Tree scheme for dense stellar systems", The 3rd AICS international Symposium, 28 Feb – 1 Mar 2013

3. Masaki Iwasawa, "Particle-Particle Particle-Tree scheme for dense stellar systems" HPCI

Strategic Program Field5 Symposium, 5-6 Mar 2013

(5)   Patents and Deliverables
     -None

(6)   Awards
Gordon Bell Prize, Tomoaki Ishiyama, *Keigo Nitadori, *Junichiro Makino, SC12, Salt Lake City USA,   15th Nov. 2012

12. Computational Climate Science Research Team

12.1. Team members

Hirofumi Tomita (Team Leader)

Shin-ichi Iga (Research Scientist)

Yoshiyuki Kajikawa (Research Scientist)

Seiya Nishizawa (Research Scientist)

Hisashi Yashiro (Research Scientist)

Yoshiaki Miyamoto (Postdoctoral Researcher)

Tatsuya Seiki (Postdoctoral Researcher)

Tsuyoshi Yamaura (Postdoctoral Researcher)

Yousuke Sato (Postdoctoral Researcher)

Ryuji Yoshida (Research Associate)

Mamiko Hata (Technical Staff)

Hiroaki Miura (Visiting Researcher)

12.2. Research Activity

In this research team, a pioneering research, which suggests the direction of future climate simulation, will be conducted. In order to raise the reliability of climate model more than the current status, we aim to construct a climate model based on more theoretically physical principles.

Such a model needs tremendously large computer resources. Therefore, it is necessary to design the model to pull out the capability of computers as much as possible. Recent development of supercomputers has a remarkable progress, however, new numerical techniques may be needed under the collaboration of hardware research and software engineering for effective use of them on the future HPC, including K computer.

For the above research achievement, our team is cooperating with the computational scientists in other fields and computer scientists. We enhance the research and development including effective techniques and make a next-generation climate model. Now, establishment of the above basic and infrastructure research on K Computer is required. This kind of research also leads to post K computer or subsequent ones. we have been continuing to conduct three ongoing projects and started two projects from this fiscal year.

1. Construction of a new library for climate study:

   We have proposed the subject "Estimation of different results by many numerical techniques and their combination" as a synergetic research to MEXT in 2011 through the discussion with the Strategic 5 fields (SPIRE).

2. Grand challenge run for sub-km horizontal resolution run by global cloud-resolving model:

In order to achieve an outstanding simulation on K computer in climate field, our team are conducting the simulation with super-high resolution This work are done in cooperation with the SPIRE3.

3. Feasibility study of Exa-scale computing using the general circulation model:

The project of G8 Research Councils Initiative "ICOMEX" has been started from 2011 autumn. Through this project, a part of our team does the feasibility study of Exa-scale computing by the global cloud resolving model and conduct the inter-comparison between the existing icosahedral models.

4. Feasibility study to the future HPCI:

In order to clarify what can be contributed from computational science to the socio/scientific field, "the Feasibility Study to the future HPCI" funded by MEXT has started from this fiscal year. RIKEN/AICS are now leading the investigation of contribution from the application side. The executive office was established in our team. We are organizing the application community of computational sciences.

5. Disaster prevention research in establishment of COE project:

Hyogo-Kobe COE establishment project has accepted 5 subjects in the last year. One of subjects is "the computational research of disaster prevention in the Kansai area". In this subject, one of sub-subjects is "Examination of heavy-rainfall event and construction of hazard map", which our team is responsible of.

12.3. Research Results

Construction of a new library for climate study:

We are working on research and development of a library for numerical models in fluid dynamical field especially in meteorological field. We examine feasibility of numerical scheme and methods and develop new ones which are suite on massive parallel computers especially K computer. In order to validate the schemes and test their performance in atmospheric simulations, we are developing an atmospheric large-eddy simulation model. Using this model, we performed standard benchmark test cases from ideal one to realistic one, such as the gravity current experiment (Straka et al. 1993), the squall line experiment (Redelsperger et al. 2000), the stratocumulus experiment (Stevens et al. 2005) and so on. We obtained reasonable results in comparison with results in previous studies, and then confirmed validity of schemes implemented in our model. Figure 1 is a result of gravity current experiment with 1.56125m resolution. A fractal shape structure of spiral due to Kelvin-Helmholtz instability can be seen. Realistic structure of cold pool, cumulus, and velocity is simulated in a 50m-resolution experiment on squall line (Fig. 2). Figure 3 is a result of a high-resolution stratocumulus experiment and it shows that it well simulate features of stratocumulus observed in the real atmosphere. It is expected that unknown processes, such as its transition to shallow cumulus,

would be clear with such high resolution experiments. High-resolution experiment on Martian planetary boundary layer for a planetary exploration project is going on using this model with Center for Planetary Science and researchers of planetary science. Our proposal on this study was accepted for general use of K computer by HCPI (project id: hp120076). Heavy rain simulation in urban area for preventing disaster is also started with Hyogo/Kobe local government, Kyoto University, and Kobe University.
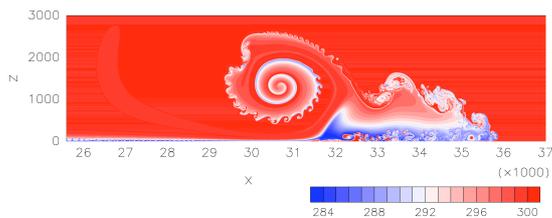

Figure 1: Potential temperature at time=570sec in a gravity current experiment with 1.5625m resolution.
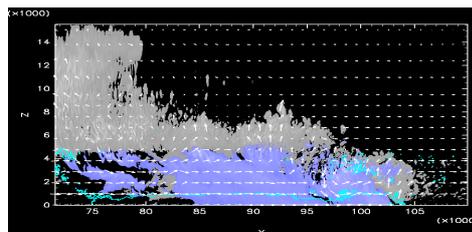

Figure 2: Horizontal-vertical cross section of rain water content (purple), othere water content (gray), temperature deviation from initial value (contour), and wind velocity (vector) in a squall
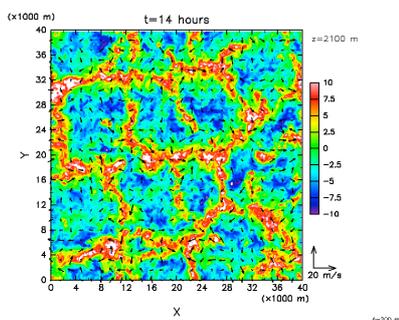

Figure. 4, Horizontal structure of convective cell at height of 2.1km in a Marian planetary boundary layer experiment. Color tone and vector show vertical velocity and horizontal velocity,
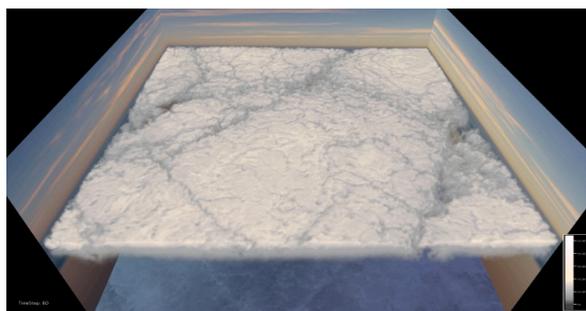

Figure 3: Could water in a stratocumulus experiment with 5m isotropic resolution.

Adding to these activities, we started collaboration with almost all major atmospheric model developing groups in Japan including Japan Meteorological Agency in developing a common basic library and environment for atmospheric models. Purpose of this activity is corporation in development of numerical code and sharing problems and knowledge for future atmospheric simulations. We are leading this activity, and held some meetings and workshop on this activity as listed below:

1. Meeting on atmospheric models, May 2012, Tokyo
2. Workshop on data analysis and numerical calculations on geophysical fluids – Current status and future plan of atmospheric/climate models in Japan -, Dec. 2012, Nagoya
3. Meeting on common basic library and environment for atmospheric models, Mar. 2013, Tokyo

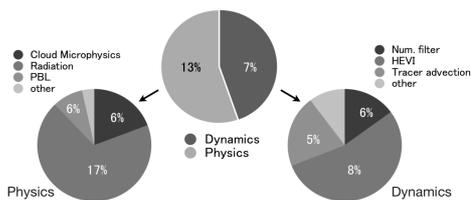**Grand challenge run for sub-km horizontal resolution run by global cloud-resolving model:**

Figure 5 Detail of time and efficiency for each major component of NICAM. The size of each pie is proportional to the computational time. Each percentage represents performance efficiency.
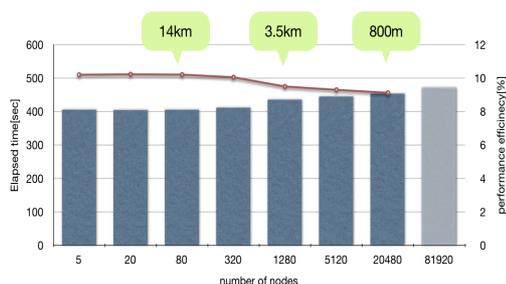

Figure 6: Weak scaling results of NICAM on the K computer. Line represents performance efficiency and Bars are elapsed time for 40 steps simulation.

Optimization of NICAM on the K computer

The optimization of NICAM on the K computer was carried out in collaboration with our team and application development team. We made cache optimization for stencil operators at first. Despite the efficiency of more than 10% was obtained in each kernel, total application performance was improved only 1%. Then we identified the part where time-consuming (large elapse time with less computation) by inserting a large number of floating-point counter and the time counter. As a result of these works, we obtain the total efficiency of about 10%. Figure 5 shows the detail of efficiency and elapse time in each major component. Figure 6 shows the result of weak scaling. It remains in the performance efficiency of ~1% reduction when we execute the model with more than 10000 nodes (80000 cores). We have good results for the almost full-node (81920 nodes) experiment. The performance of NICAM on the K computer obtained as a result of these optimizations enables the simulation such as long-term calculation, ensemble experiments, and ultra-high resolution experiments.

Grand Challenge run

We have first succeeded in conducting a Grand Challenge simulation, which includes global simulation with extremely high horizontal resolution (0.8 km) and 96 vertical levels, and simulations with varying the resolution from 30 km up to 0.8 km. We investigated the characteristic of deep moist convection in each simulation. Deep moist atmospheric convection which horizontally extends from 1 to 10 km is the element of cloudy weather disturbances such as tropical cyclones. Because of its essential importance, the convection has been modeled with special attention. However, it has been difficult to explicitly simulate the convection in global circulation models due mainly to resolution and computer performance. We used the 6 different global simulations whose horizontal resolutions is 30 km, 14 km, 7 km 3.5 km, 1.7 km and 0.8 km respectively. We defined uniform method to detect the deep convection area and convection core grid and applied to each simulation. It was revealed that the characteristics of the simulated deep moist convection (upward velocity, total number, areal ratio of convection core, and distance to the nearest convection core) were dramatically changed between the 3.5 km and 1.7 km resolutions. Thus, the present results suggest that the spatial resolution needs to be less than about 2.0 km to resolve the deep convection(Fig.7).

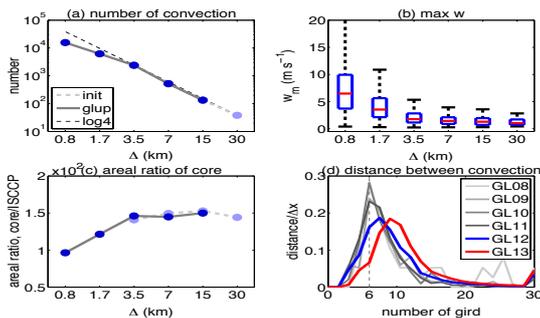Figure 7: Resolution dependences of convection characteristics: (a) the number of convection, (b) the maximum vertical velocity, (c) the ratio of the area of convection core to that of convective grids, and (d) the grid distance to the nearest convection. The thin—dashed line in (a) indicates log x4 as a reference. GL08 denotes 30 km horizontal resolution, while GL13 indicates 0.8 km resolution.

100

Improvement of icosahedral grid and its family:

For stable, accurate, and cost-effective simulation in the icosahedral grid, smoothness and homogeneity are important grid properties. From this viewpoints, we investigated the grid properties and found that the stability of the spring dynamics grid decreases as the resolution increases using the standard method. To avoid this instability, the natural spring length should be shortened, while this decreases the grid homogeneity. To overcome these disadvantages, we devised a new grid-generation method that combines the spring dynamics method with a zero spring natural length and transformation by a smooth analytical function. Using this method, we found that the grid performance (homogeneity) improved at most resolutions, with the greatest increase at high resolution. We examined the grids using test case 1 of D. L. Williamson et al. (1992) and found that the proposed grid worked well in terms of accuracy and tolerability against CFL constraints.

Further, in pursuit of a computational resource cost-effective atmospheric general circulation model, a grid enhanced in the tropics was developed. The tropics-enhanced grid has about 60% of the number of grid points as the icosahedral grid. Conducting the aqua planet experiment by a quasi-uniform icosahedral grid and the grid enhanced in the tropics, we compared these results.

ICOMEX project
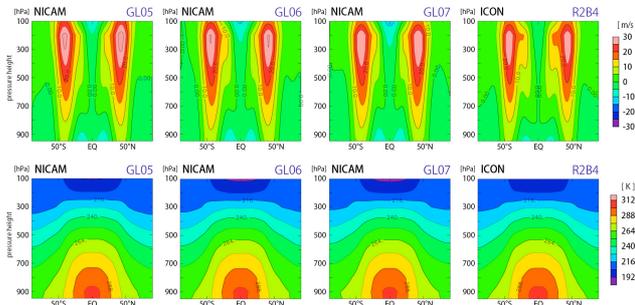
Figure 8. Zonal mean latitude-vertical profile of zonal wind and temperature for NICAM and ICON: shown values are time averaged among 1000 days after 300 days spin-up. For NICAM, horizontal resolutions for GL05, GL06, and GL07 are 240 km, 120 km, and 60 km, respectively. A horizontal resolution for ICON R2B4 is 160 km. Positive zonal wind means westerly wind.
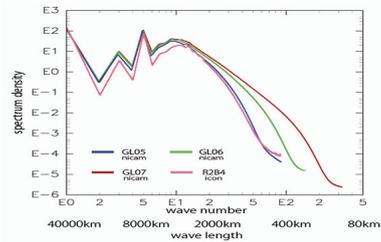
Figure 9: kinetic energy spectrum at 10 km height for NICAM and ICON: the values are calculated using u, v, and w component, and time averaged for 500 days. For NICAM, horizontal resolutions for GL05, GL06, and GL07 are 240 km, 120 km, and 60 km, respectively. A horizontal resolution for ICON R2B4 is 160 km.

The ICOsahedral-grid Models for EXascale Earth system simulations (ICOMEX) is the consortium for the climate models development toward the exascale computing. Participated are NICAM (Japan), ICON (Germany), MPAS (UK and US), and DYNAMICO (France) model teams. The Japan team works on the model inter-comparison to be synergistic among working groups. Although all the participated models use the icosahedral-grid, the discretization methods are different. We focus on both physical and computational performance.

We prepared three experiment settings. As the first step, to check physical performance, we prepared

experiment setting for three test cases, which are statistical climate test, deterministic baroclinic wave test, and realistic climate test. Test production has been started for NICAM, ICON, and DYNAMICO.

Held and Suarez (1994) test case was carried out in NICAM and ICON. The profiles of temperature and zonal wind are shown in Figure 8. Temperature profiles and westerly jet were simulated reasonably both in NICAM and ICON. Figure 9 is power spectrum of kinetic energy at 10 km height. It is also reasonable that a spectrum by simulated in higher resolution has longer tail for high frequency side than spectrum tail in lower resolution.

Jablonowski and Williamson (2004, 2006) test case which is a deterministic test of baroclinic wave has been performed by using NICAM, ICON, and DYNAMICO. Wave shape and its phase are reasonable for all three models.

Feasibility study to the future HPCI:

FY2012, 5 general meetings were held and extraction of social/science subjects, which should be resolved in the next generation HPC. We also discussed about them with the other communities. The report can be found in http://hpci-aplfs.aics.riken.jp/.

Hoygo-Kobe COE establish project:

In this year, we launched the consortium of the computational research of Disaster prevention for Kansai area with Kyoto University and Kobe University, based on the Hyogo-Kobe COE. The kickoff meeting was held in AICS in January 2013.

12.4. Schedule and Future Plan

In the next year, we will continue to construct the numerical library for K computer and release the 1st version of library until the end of FY2013. At the same time , we will give an insight into what kind of the time integration method is promising on K computer and future HPC from the viewpoints of computational and physical performances. Through this project, we will organize and lead the meteorological numerical community for common library towards the post-Peta scale computing.

Grand challenge run by NICAM will be also continued in cooperation with 3rd Strategic Field Project. The statistical properties of deep convection and convergence of grid refinement will be investigated and clarified in detail.

In the ICOMEX project, we also continue to do model inter-comparison. So far, all participated model are ready to compare each other. Focusing on the physical performance, four models are inter-compared through such as aqua planet experiment.

On the Feasibility study, the science roadmap will be further brushed up with inside/outside researchers. The office of this project in our team will continue to organize the meeting and enhance the discussion. The estimation of the systems, which is proposed by 3 system-design teams will be a mission of this project. This will be performed with 3 system-design teams.

On the COE establishment project, we have a plan to use the SCALE library. In the next year, we add several components such as city-model and start to research the mechanism of heavy-rainfall in Kansai-area with collaborated organization.

12.5. Publication, Presentation and Deliverables

(1) Journal Papers

1. Oouchi, K., H. Taniguchi, T. Nasuno, M. Satoh, H. Tomita, Y. Yamada, M. Ikeda, R. Shirooka, H. Yamada, K. Yoneyama, 2012: A prototype quasi real-time intra-seasonal forecasting of tropical convection over the warm pool region: a new challenge of global cloud-system-resolving model for a field campaign. Nova Science Publishers, Inc., Eds. K. Oouchi and H. Fudeyasu, pp.233-248.

2. Yoshizaki, M., Yasunaga, K., Iga, S.-I., Satoh, M., Nasuno, T., Noda, A. T., Tomita, H., 2012: Why do super clusters and Madden Julian Oscillation exist over the equatorial region? SOLA, 8, 33-36, doi:10.2151/sola.2012-009.

3. Noda, A. T., Oouchi, K., Satoh, M., Tomita, H., 2012: Quantitative assessment of diurnal variation of tropical convection simulated by a global nonhydrostatic model without cumulus parameterization. J. Clim., 25, 5119-5134.

4. Satoh, M., Iga, S., Tomita, H., Tsushima, Y., Noda, A.T., 2012: Response of upper clouds due to global warming tested by a global atmospheric model with explicit cloud processes. J. Clim., 25, 2178-2191.

5. Dirmeyer, P. A., Cash, B. A.,Kinter III, J. L., Jung, T., Marx, L., Satoh, M., Stan, C., Tomita, H., Towers, P., Wedi, N., Achuthavarier, D., Adams, J. M., Altshuler, E. L., Huang, B., Jin, E. K., and Manganello, J., 2012: Simulating the diurnal cycle of rainfall in global climate models: Resolution versus parameterization. Clim. Dyn., 39, 399-418, DOI10.1007/s00382-011-1127-9.

6. Miyamoto, Y. and T. Takemi, 2013: A transition mechanism for spontaneous intensification of tropical cyclones. J. Atmos. Sci., 70, 112-129.

7. Fudeyasu, H. and Y. Miyamoto, 2013: Intensification phase and steady state, *Meteorological Research Note*, 226.

8. Yoshizaki, M., S. Iga, and M. Satoh 2012:Eastward-propagating property of large-scale precipitation systems simulated in the coarse-   resolution NICAM and an explanation of its formation.: Scientific Online Letters on the Atmosphere , 8, pp.21-24,

9. Yoshida R., and H. Ishikawa, 2013: Environmental factors contributing to tropical cyclone genesis over the western North Pacific. Mon. Wea. Rev., 141, 451–467.

10. Yamaura, T. and T. Tomita, 2012: Covariability between the Baiu precipitation and tropical cyclone activity through large-scale atmospheric circulation. J. Meteor. Soc. Japan, 90, 449-465.

(2) Conference Papers

-None

(3) Invited Talks

1. Tomita, H.: SCALE toward the library of meteorological applications suitable to the future super Toward Global LES, 5th International Workshop on Cloud-Resolving Global Modelling, 13-15th June 2012 (invited)

2. Tomita, H., Japanese Post-Peta Planning and Feasibility Research, Application, 18th International Exa-scale Software Project, 11-13 April 2012 (invited)

3. Tomita, H. Research of tropical meteorology and climate using K computer, Singapore-Japan High Performance Computer Workshop, Singapore, 27-28 Feb.2012 (invited)

4. Yashiro, H., NICAM.12: Recent Performance on the K Computer and Further Development toward Post Peta-scale Computing (Invited), 2012 KIAPS International Symposium, Seoul, Korea, Nov. 2012.

(4) Posters and presentations

International and Domestic conference/symposium/workshop

1. Tomita, H., S. Nishizawa, H. Yashiro SCALE-LES: Strategic development toward the future global LES, 1st International Conference on Frontiers in Computational Physics: Modeling the Earth System, Boulder, CO, USA 16 - 20 December 2012

2. Tomita, H: SCALE-LES: Strategic development of large eddy simulation suitable to the future HPC, Solution of Partial Differential Equations on the Sphere (PDEs on the sphere), 24-28 September, 2012, Cambridge

3. Tomita, H.: Development of moist-LES model in RIKEN/AICS, The 14th international specialist meeting on the next generation models on climate change and sustainability for advanced high performance computing facilities Hawaii, 12-15 Mar., 2012

4. Tomita, H.: Present Status of K Computer and activity toward the Exa-Scale Computing, The 14th international specialist meeting on the next generation models on climate change and sustainability for advanced high performance computing facilities Hawaii, 12-15 Mar., 2012

5. Sato, Y., H.Yashiro, S. Nishizawa, Y.Miyamoto, H. Tomita, and Team-SCALE : Development of SCALE-LES3 model and numerical simulations of shallow clouds by the model, *Second International Workshop on Nonhydrostatic Numerical Models*, Sendai, Japan, November, 2012

6. Sato, Y., H. Yashiro, S. Nishizawa, Y. Miyamoto, H. Tomita: Development of SCALE-LES3 model and numerical simulation of shallow clouds by the model, *1st International conference on Frontires in computational physics: Modeling the earth system*, O15, Boulder, CO, USA, December, 2012

7. Sato, Y., H. Yashiro, S. Nishizawa, Y. Miyamoto, Team-SCALE, and H. Tomita: Numerical simulations of shallow clouds by using SCALE-LES, Autumn Meeting, Meteorological Society of Japan, Sapporo, 3-5, Oct., 2012.

8. Miyamoto, Y., H. Yashiro, S. Nishizawa, Y. Sato, H. Tomita and Team SCALE, 2012: Impacts of numerical grid on atmospheric boundary-layer turbulence in large eddy simulations using a fully compressible model., *1st International Conference on Frontiers in Computational Physics,* Boulder, Colorado, U.S.A..

9. Miyamoto, Y. and T. Takemi, 2012: A transition mechanism for the spontaneous axisymmetric intensification of tropical cyclones.. *2012 AGU fall meeting, San Francisco*, U.S.A..

10. Miyamoto, Y., H. Yashiro, S. Nishizawa, Y. Sato, H. Tomita and Team SCALE, 2012 : Impacts of numerical grid on atmospheric boundary-layer turbulence in large eddy simulations using a fully compressible model. *2nd International workshop on Non-hydrostatic modeling*, Sendai, Japan.

11. Miyamoto, Y. and T. Takemi, 2012: An effective radius of the sea surface enthalpy flux for the maintenance of a tropical cyclone. *18th Conference on Air-Sea Interaction*, Boston, U.S.A.

12. Miyamoto, Y. and T. Takemi, 2012: A transition mechanism for the spontaneous axisymmetric intensification of tropical cyclones. *30th Conference on Hurricanes and Tropical Meteorology*, Ponte Vedra Beach, Florida, U.S.A..

13. Miyamoto, Y. and T. Takemi, 2012: An effective radius of the sea surface enthalpy flux for the maintenance of a tropical cyclone. *Ocean Sciences Meeting 2012*, Salt Lake City Utah, U.S.A.

14. Miyamoto, Y., H. Yashiro, S. Nishizawa, Y. Sato, H. Tomita and Team SCALE, 2012 : The effects of grid shape on boundary-layer turbulence above a heated surface. Meteorological Society of Japan, Sapporo, Oct. 4th, 2012.

15. Miyamoto, Y., 2012 :Maximum potential intensity theory of tropical cyclones including the ocean cooling process: A discussion on the nondimensional parameter. Meteorological Society of Japan, Sapporo, Oct. 4th, 2012.

16. Miyamoto, Y., T. Takemi, 2012 : The trigger of spontaneous axisymmetric intensification of tropical cyclones Meteorological Society of Japan, Tokyo, May 20th, 2012.

17. Iga, S., H. Tomita, M.Tsugawa 2012, A generalization and combination of map projection on a sphere and its application to global grid system. The 14th international specialist meeting on the next generation models of climate change and sustainability for advanced high performance computing facilities. (2012.03.12-15, Maui, Hawaii,)

18. Yoshida R., 2012: A development process of the tropical disturbance observed in PALAU2010 for understanding tropical cyclogenesis. *30th Conference on Hurricanes and Tropical Meteorology*, Ponte Vedra Beach, Florida, U.S.A.

19. Yoshida R., and H. Tomita, 2012: G8 ICOMEX: Introduction & preliminary result. The 14th

international specialist meeting on the next generation models on climate change and sustainability for advanced high performance computing facilities Hawaii, 12-15 Mar., 2012

20. Yoshida R., and H. Tomita, 2012: NICAM presentation and evolution, G8 ECS workshop, 6-7 March, 2012 at Aachen, Germany

21. Yoshida R., and H. Tomita, 2012: G8 call: ICOMEX project - the introduction, G8 ECS workshop, 6-7 March, 2012 at Aachen, Germany

22. Yoshida R., and H. Tomita, 2012: An Inter-Comparison of Icosahedral Climate Models on the G8 Call: ICOMEX Project. Solution of Partial Differential Equations on the Sphere (PDEs on the sphere), 24-28 September, 2012, Cambridge

23. Yoshida R., H. Tomita, M. Satoh: An inter-comparison of icosahedral grid models - G8 Call:ICOMEX Project, 2012 Autumn Meeting, Meteorological Society of Japan, Sapporo, 3-5, Oct., 2012.

24. Seiki, T., M. Satoh, T. Nakajima, and H. Tomita, 2012: Aerosol effects of the condensation process on a tropical squall line simulation. 16th International Conference on Clouds and. Precipitation, Leipzig, Germany

25. Seiki, T., D. Goto, K. Suzuki, M. Satoh, and H. Tomita, 2012: Modeling of wet deposition process coupled with a double moment bulk cloud microphysics scheme, 11th AEROCOM Workshop, Seattle, USA

26. Yamaura, T. and T. Tomita, 2012: Subseasonal change in interannual variations of the Baiu precipitation. AGU Fall Meeting 2012, 3-7 December, San Francisco, CA, USA.

27. Yamaura, T. and T. Tomita, 2012: Covariability between the Baiu precipitation and tropical cyclone activity through large-scale atmoshperic circulation. AOGS-AGU 2012, AS01-A007, 13-17 August, Singapore.

28. Yamaura, T., T. Tomita, 2012: Subseasonal change in the interannual variability of the Baiu precipitation. Meteorological Society of Japan 2012 Fall meeting, P180, 3-5 October 2012, Hokkaido University, Hokkaido.

29. Yamaura, T., T. Tomita, 2012: Covariability between the Baiu precipitation and tropical cyclone activity through large-scale atmospheric circulation. Meteorological Society of Japan 2012 Spring meeting, B166, 26-29 May 2012, Tsukuba International Congress Center, Tsukuba.

30. Yamaura, T., T. Tomita, 2012: Covariability between the Baiu precipitation and tropical cyclone activity through large-scale atmospheric circulation. Japan Geoscience Uniton 2012 Annual meeting, AAS23-P11, 20-25 May 2012, Makuhari Messe International Convention Complex, Chiba.

31. Kajikawa, Y., Wang B. and H. Murakami, 2012: South China Sea summer monsoon onset simulated by the high-resolution MRI-AGCM, AGU Fall Meeting 2012, 3-7 December, San Francisco, CA, USA.

32. Kajikawa, Y., Wang B. and H. Murakami, 2012: South China Sea summer monsoon onset simulated by the high-resolution MRI-AGCM, Meteorological Society of Japan 2012 Fall meeting, P180, 3-5 October 2012, Hokkaido University, Hokkaido.

33. Tomita, H., Introduction of Japanese activities toward the Exa-scale computing, The workshop for next-generation of climate models and knowledge discoveries through the extreme high performance simulations and big data, Berkeley, CA, USA, 2012

34. Nishizawa, S., Yashiro,H., Sato,Y.,Miyamoto,Y., Tomita,H. and Team SCALE, Research and Development of Common Basic Library and Environment for Weather and Climate Prediction Models, The workshop for next-generation of climate models and knowledge discoveries through the extreme high performance simulations and big data, Berkeley, CA, USA, 2012

35. Nishizawa. S., H. Yashiro, Y. Miyamoto, M. Odaka, Y. Takahashi, Y.-Y. Hayashi, H. Tomita, S. Takehiro, M. Ishiwatari, K. Nakajima, Y. Sato, K. Sugiyama, Team SCALE, and GFD Dennou Club: A large-eddy simulation experiment on turbulence in Martian planetary boundary layer, 2012 Autumn Meeting of Meteorological Society of Japan, Sapporo, Japan, October, 2012

36. Nishizawa. S., H. Yashiro, Y. Miyamoto, M. Odaka, Y. Takahashi, Y.-Y. Hayashi, H. Tomita, S. Takehiro, M. Ishiwatari, K. Nakajima, Y. Sato, K. Sugiyama, Team SCALE, and GFD Dennou Club: A large-eddy simulation experiment on turbulence in Martian planetary boundary layer, 2012 Annual Meeting of the Japanese Society for Planetary Sciences, Kobe, Japan, October, 2012

37. Yashiro,H., Tomita,H. and Satoh,M., NICAM simulations on the K computer: recent performance and activities toward to the exascale computing, The workshop for next-generation of climate models and knowledge discoveries through the extreme high performance simulations and big data, Berkeley, CA, USA, 2012

38. Sawada,M., Miyagawa,T., Nakano,M., Yamaura, T., Noda,A.T., Kajikawa,Y., Yamada,Y., and Satoh,M., Study of extended-range predictability using global cloud system resolving model NICAM, The workshop for next-generation of climate models and knowledge discoveries through the extreme high performance simulations and big data, Berkeley, CA, USA, 2012

 (5) Patents and Deliverables
    -None

13. Complex Phenomena Unified Simulation Research Team

13.1. Team members

Makoto Tsubokura (Team Leader)

Chung-gang Li (Postdoctoral Researcher)

Keiji Onishi (Research Associate)

Ryoichi Kurose (Visiting Researcher)

Gakuji Nagai (Visiting Researcher)

Kei Akasaka (Visiting Researcher)

Yuri Iida (Assistant)

13.2. 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 cutting-edge 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.

13.3. Research Results and Achievements

13.3.1. Feasibility study of the building-cube method for complicated geometry

As a candidate of unified data structure for complicated and coupled phenomena, we focused on the building-cube method (BCM) proposed by Nakahashi[1]. The basic strategy of mesh generation by BCM is as follows: (1) Target flow field is decomposed into cubes of various sizes with their side length given as the exponent of 2 with respect to the minimum side length as one; (2) Each side of the cubes with the same size is subdivided at even intervals and uniform Cartesian mesh is generated in each cube. It should be noted that the number of grids is the same for all cubes with different sizes. The advantages of the BCM against the conventional unstructured grid used in the CFD of industrial applications are: Firstly, the data format is fully structured, making it easy to handle the hierarchical cash memories, and thus higher peak performance for single core is expected; Secondly, by allocating the same number of cubes for each core, exactly the same load balance including core to core communication is achieved, and thus higher parallel performance is expected. On the other hand, the disadvantage of the Cartesian mesh including the BCM is the treatment of the curved surface typically observed in industrial products. In this study, in addition to the conventional immersed boundary method to treat the curved surface by the voxel grid, additional methods are implemented to re-construct the solid surface information for flow simulation including the treatment of thin or thick-less geometry data. In fact these new methods turn the disadvantage of the solid body treatment in the Cartesian mesh into an advantage to the unstructured grid. By using the methods we could generate the numerical mesh by BCM without modifying the data defect in CAD data, such as little gaps or overlaps between two parts or unnecessary tapped hole on the surface.

The feasibility of the BCM including solid-surface treatment was tested in the real CAD data utilized in automotive industry, as shown in Fig. 1. Some data defections observed in the CAD data are indicated in Fig.2, in which the regions with red and cyan color show little gaps and overlaps between two parts, respectively. The number of the defections amounts to more than 1,000 places, and requires modification by hands if we generate conventional unstructured grids. Typically a couple of days are required for the modification in real industrial processes. On the other hand, we have confirmed that it took only less than 10 minutes including the automatic surface modification to generate BCM mesh of about 150 million cells, as shown in Fig. 3. In the mesh generation, the size of the analysis domain is given as 40m by 10m by 10m, which is divided by 87,558 cubes, and each cube is subdivided by 8x8x8 cells. In this case, the surface resolution is about 5mm on the vehicle surface.

Flow structures and the magnitude of flow velocity around the vehicle are visualized in Fig.4. The simulation was conducted on the K-computer using 512 CPUs. It took only about 4 wall-clock hours to obtain the result, including the mesh-generation time. The feasibility study has been successfully finished by validating the BCM for engineering CFD.
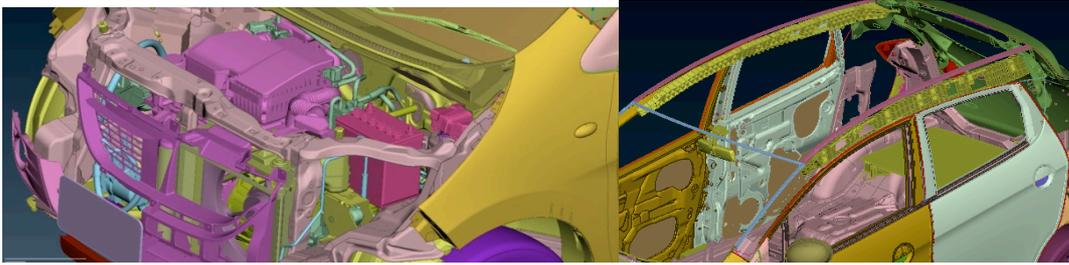
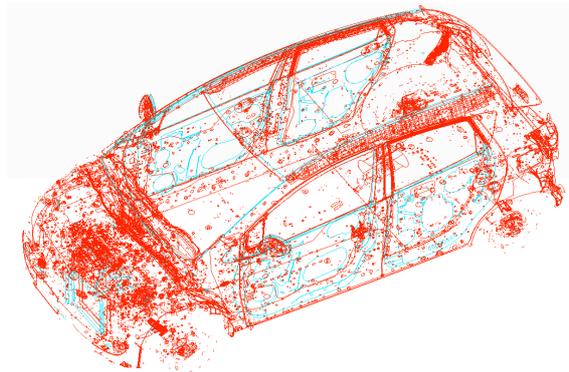Fig. 1 CAD data of a full-scale road vehicle used in an industrial process.

Fig. 2 Data defecting points in a CAD (red: gap, and cyan: overlap of two parts).
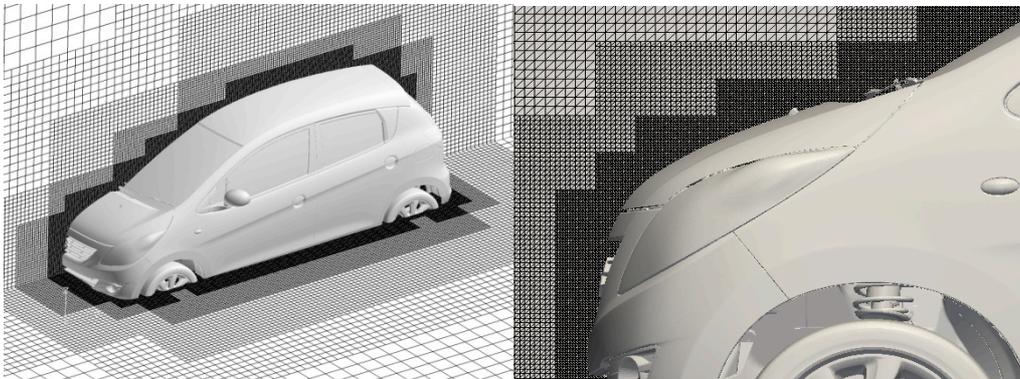

Fig. 3 BCM mesh generated around a full-scale vehicle using about 150 million cells.
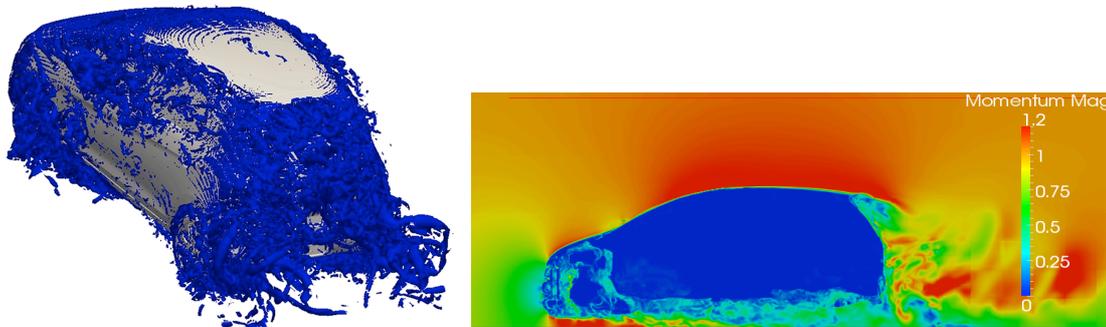

Fig. 4 Flow structures (left) and the magnitude of flow-velocity around the vehicle.

110

13.3.2 Feasibility study of a pre-conditioning compressible simulation for unified low to moderate Mach number turbulent flow

For the purpose of unifying the simulation, the fluid compressibility, turbulent effects and heat transfer should be taken into consideration simultaneously. In such kind of sever situation, the program which could only cope with the incompressible flow would be restricted for the practical applications. In order to solve the problem mentioned above, the preconditioning method which can be used on turbulent compressible flow in the full speed regions have been investigated and developed in the presently study.

The Roe scheme [2], Weiss and Smith preconditioning method and dual time stepping [3] have been implemented because of their sophisticated applicability on the transient state problems. For the sake of investigating the validation of this method on the low speed compressible turbulent flow ($M = 0.005$), the channel flow at $\mathrm{Re}_\tau = 180$ has been performed and all the simulation conditions are based on the direct numerical simulation based on the spectral method for incompressible flow conducted by Kim et al [4].

Figure 8 are the instant contour of the velocity magnitude and shows several noticeable turbulent characteristics. In the $x_1 x_2$ plane, the flow field is unstable and contains different scales of the velocity magnitude near the wall. These phenomena are due to the turbulence injection from the wall. From the $x_2 x_3$ plane, the injection can be observed more clearly near the wall. Besides, the streakline is also an important characteristic for the turbulence. In the $x_1 x_3$ close the wall, there are several clear streaklines which can be easily distinguished.

Based on the present results mentioned above, there are several conclusions listed below. Firstly, this method can be used on very low Mach region and the result is in good agreement with the incompressible flow method. Secondly, it should be recognized that most of industry applications belongs the turbulence. This method also shows it has good capability on solving turbulence flow. Thirdly, preconditioning would change the temporal term and the governing equation is not suitable for transient state problems. Dual time stepping overcomes this disadvantage. From the turbulence statistical results, it can be known that the Roe scheme, Weiss and Smith preconditioning method and dual time stepping can be used on transient state problems. Therefore, this program will be a powerful tool on unifying the simulation method.

Besides, this method will be also a promising candidate for our next target-computational aeroacoustic (CAA). Basically, the study of aeroacoustic noise involves two academic fields. One is the compressible turbulent flow and the other is aeroacoustics. Usage of the results of the disturbance of density, pressure and velocity obtained from the compressible turbulent flow as an aeroacoustic source substitutes into the appropriate governing equations for example, Lighthill or Ffowcs Williams and Hawkings equations to calculate the noise propagation.

Due to the instinct of the compressible flow program, this method has the potential to accurately capture the density variation and turbulent fluctuations which are the main aeroacoustic

source in the flow field. Therefore, the present program can be used to calculate the aeroacoustic source in the practical applications of controlling noise.
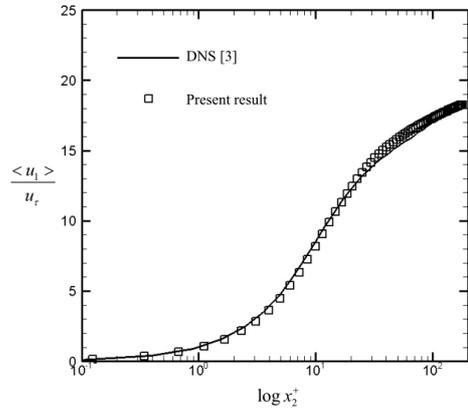

Figure 5. The distributions of mean velocities
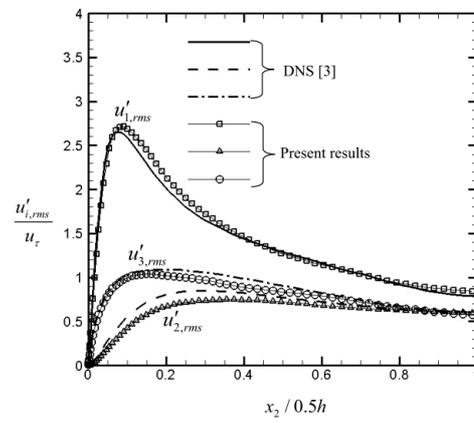
Figure 6. The distributions of turbulent intensities
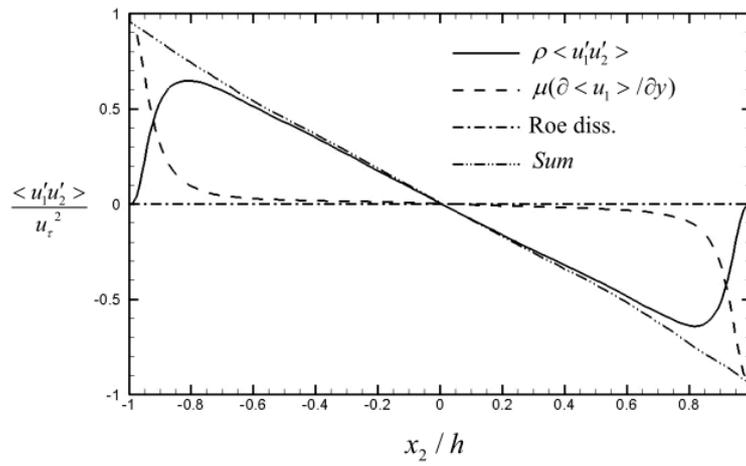
Figure 7. The distributions of Reynolds stress
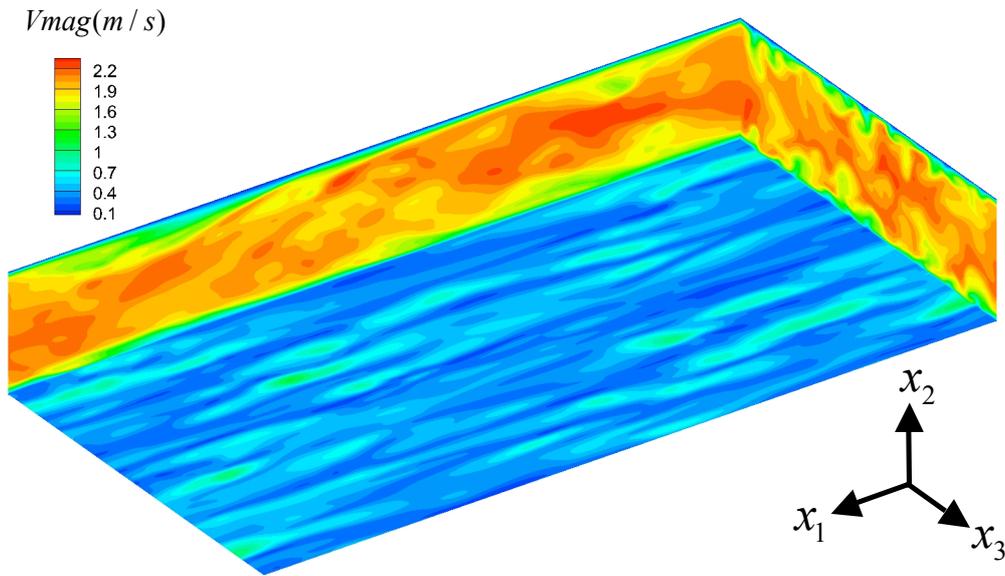
Figures 8. The instant contour of the velocity magnitude

[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] J. Kim, P. Moin and R. Moser, Turbulence statistics in fully developed channel flow at low Reynolds number, J. Fluid Mech. 177 (1987) 133-166.

13.4. Schedule and Future Plan

(1)Five-year objectives and goals toward 2017

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

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

(2)Long-term objectives

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

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

(3)Time schedule

	2012	2013	2014	2015	2016	2017
Proposal of the project	Interview to the industry and feasibility study					
		Making specification list for the development				
Building light libraries		Library development	Porting guideline			
		Application development				
Development of the coupling algorithms for the PETA-scale computing		Development of the scaling algorithms				
			Development of the coupling algorithms			
Validation studies		PETA-scale applications			Performance test of the post PETA-scale applications	

13.5. Publication, Presentation and Deliverables

(1) Journal Papers
    -None

(2) Conference Papers
    -None

(3) Invited Talks
1. Makoto Tsubokura: Next-generation design system for aerodynamics/thermal management for road vehicle development, K-computer symposium 2012 (15th, June, 2012 at Univ. Kobe, Shin-Kokusaikaigijou) in Japanese
2. Makoto Tsubokura: Vehicle-aerodynamics development using supercomputer and challenge for the new mystery of aerodynamics, Supercomputer K wo shiru tsudoi in Kanazawa(4th, August, 2012 at Kanagawa Bunkyoukaikan) in Japanese
3. Makoto Tsubokura: Vehicle-aerodynamics development using supercomputer and challenge for the new mystery of aerodynamics, Supercomputer K wo shiru tsudoi in Kanazawa(4th, August, 2012 at Kanagawa Bunkyoukaikan) in Japanese

(4) Posters and presentations
    -None

(5) Patents and Deliverables
    -None

14. HPC Programming Framework Research Team

14.1. Team members

Naoya Maruyama (Team Leader)

Motohiko Matsuda (Research Scientist)

Soichiro Suzuki (Technical Staff)

Mohamed Wahib (Postdoctoral Researcher)

Michel Müller (Technical Staff)

14.2. Research Activities

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

1) Large-Scale Data Processing with KMR

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

2) Physis: An Implicitly Parallel Stencil Computation Framework

Physis is a framework for stencil computations that is designed for a variety of parallel computing systems with a particular focus on programmable GPUs. The primary goals are high productivity and high performance. Physis DSL is a small set of custom programming constructs, and allows for very concise and portable implementations of common stencil computations. A single Physis program runs on x86 CPUs, NVIDIA GPUs, and even clusters of them with no platform-specific code. This software consists of a DSL translator and runtime layer for each supported platform. The translator automatically generates platform-specific source code from Physis code, which is then

compiled by a platform-native compiler to generate final executable code. The runtime component is a thin software layer that performs application-independent common tasks, such as management of GPU devices and network connections.

14.3. Research Results and Achievements

14.3.1. Large-Scale Data Processing with KMR

Our major achievements with KMR consist of its basic design and the first prototype implementation. The design of KRM is similar to Hadoop, which is a popular MapReduce implementation in Java, but our implementation is completely different. We initially considered reusing much of the Hadoop software components, but because of limited support of the Java programming language on the K computer, we define our own MapReduce as a standard C library. This allows for simpler integration of existing optimized system software components. For example, data shuffling is one of the most challenging processing phase in MapReduce because of its high communication intensity, so exploiting the maximal performance of the underlying interconnect, the Tofu network, is highly important. Our KMR is designed in a way that such optimizations for large-scale supercomputers can be transparently integrated.

14.3.1.1 Prototype Implementation and its Optimizations

The basic prototype implementation runs on both the K computer and standard cluster systems with several K-specific extensions and optimizations, including fast file reading and scalable data shuffling. The storage architecture of the K computer system consists of the global storage, which presents very large capacity (tens of peta bytes), and the local storage, which allows for higher bandwidth and lower latency than the global storage when I/O accesses by user applications exhibit spatial and temporal locality. The two storage systems are organized by the K's data staging system, however, I/O read performance with the local storage still exhibits scalability problems even with a modest number of nodes. This is often the case with MapReduce, where a large number of Mapper processes simultaneously access input data. In our KMR, this operation is tuned for the K storage architecture by limiting the read concurrency to storage systems and exploiting the inter-node data communications. This optimization effectively introduces additional data staging to the application I/O data flow, where the first staging is performed between the global and local storage systems, and the second staging is between the local storage and compute nodes. A comparative performance study can be found in Fig 1, which shows much more scalable performance than a normal I/O method. Although the additional stage complicates the overall application structure when it is implemented manually, it is completely automated in our KMR library without any user intervention.
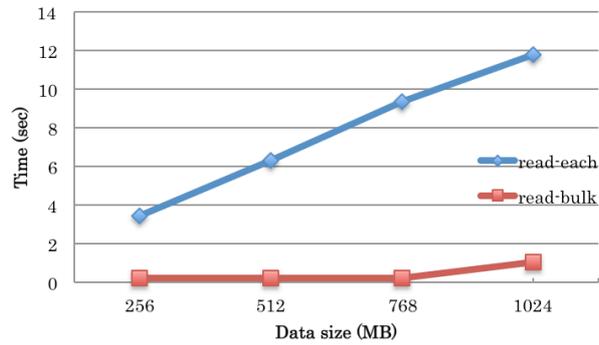
Fig. 1   Read latency comparison on 192 nodes. The blue line shows the read time when all nodes simultaneously read the data, while the red line shows the performance when only a part of the nodes load the data from the local storage, which are then transferred to the rest of the nodes by using MPI over the Tofu network.

  Another major optimization is the scalable data shuffling. Since each map operation tends to generate relatively small data to be consumed by the reduce operation, our KMR uses a collective communication algorithm proposed by Bruck et al., which performs communications in log(p) stages, where p is the number of processes. As shown in Fig. 2, the performance with our own implementation exhibits much better performance for small messages, but it quickly increases as the
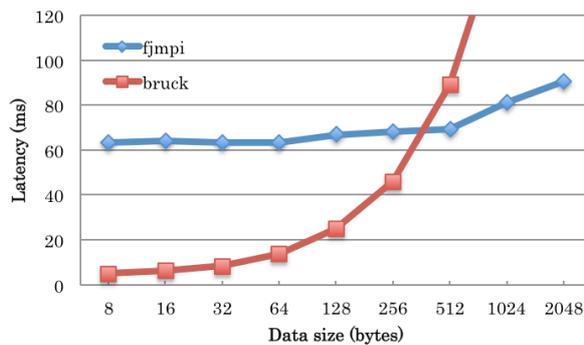
Fig. 2   Comparison of data shuffling time on 16384 nodes. The blue line shows the performance when using an all-to-all API of the Fujitsu MPI, while the red line shows the performance using the custom collective communication.

data size grows. Since the selection of communication methods have large performance impact on data shuffling, we plan to develop an intelligent mechanism that automatically choose the most efficient one depending on message sizes.

14.3.1.2 Case Study: Metagenome Sequence Analysis

As a case study, we applied KMR to metagenome sequence analysis. Sequence homology search is an important computational method in life science. Sequences similar to known amino acid sequences are searched using large-scale metagenome sequences. We have developed a MapReduce-based implementation using a homology search program called GHOSTX developed at the Tokyo Institute of Technology. We have demonstrated that a large number of compute nodes of the K computer can be used to achieve higher performance, even without parallel programming.

14.3.2 Physis: An Implicitly Parallel Stencil Computation Framework

The main achievement in the Physis framework is optimized code generation to achieve both high productivity and high performance. The Physis DSL translator now has a set of translation passes that apply a variety of generic and stencil-specific optimizations, which achieves comparable performance as hand-tuned stencil code on a GPU. Furthermore, we developed a prototype auto-tuner for Physis, which experimentally finds the best configuration of optimization passes. Detailed evaluation and extended case studies are subject of future work.

Other major achievements include modeling and implementation of scalable fault-tolerance schemes, and evaluation of new accelerator programming models. In particular, we conducted an extensive performance study of OpenACC, which is a new directive-based accelerator programming interface. Our finding suggests that it can greatly simplify programming burden, however, the performance cost compared to tuned CUDA code still needs to be addressed.

14.4. Schedule and Future Plan

Our major milestones in FY2013 are the fist release of KMR and further application case studies. The release will be freely available on the K computer with documentation and sample applications. We plan to apply the implementation to a wider variety of applications to demonstrate its effectiveness.

Our current implementation has several limitations, including lack of fault tolerance and load balancing, both of which are important challenges in large-scale machines such as K and subject of our long-term research goals.

14.5. Publication, Presentation and Deliverables

(1) Journal Papers

-None

(2) Conference Papers

1. Tetsuya Hoshino, Naoya Maruyama, Satoshi Matsuoka, Ryoji Takaki, "CUDA vs

OpenACC: Performance Case Studies with Kernel Benchmarks and a Memory-Bound CFD Application," Proceedings of the 2013 IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid 2013), Delft, the Netherlands, May 2013.

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

3. Kento Sato, Naoya Maruyama, Kathryn Mohror, Adam Moody, Todd Gamblin, Bronis R. de Supinski, Satoshi Matsuoka, "Design and modeling of a non-blocking checkpointing system," Proceedings of the 2012 ACM/IEEE conference on Supercomputing (SC'12), pp. 19:1--19:10, Salt Lake City, Utah, November 2012.

4. Kenjiro Taura, Jun Nakashima, Rio Yokota, Naoya Maruyama, "A Task Parallelism Meets Fast Multipole Methods," Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems (ScalA), Salt Lake City, Utah, November 2012.

5. Leonardo Bautista Gomez, Thomas Ropars, Naoya Maruyama, Franck Cappello, Satoshi Matsuoka, "Hierarchical Clustering Strategies for Fault Tolerance in Large Scale HPC Systems," Proceedings of the 2012 IEEE International Conference on Cluster Computng (CLUSTER), pp. 355--363, Beijing, China, September 2012.

6. Leonardo Bautista Gomez, Bogdan Nicolae, Naoya Maruyama, Franck Cappello, Satoshi Matsuoka, "Scalable Reed-Solomon-Based Reliable Local Storage for HPC Applications on IaaS Clouds," Proceedings of Euro-Par 2012, pp. 313--324, Rhodes Island, Greece, August 2012.

7. Irina Demeshko, Naoya Maruyama, Hirofumi Tomita, Satoshi Matsuoka, "Multi-GPU Implementation of the NICAM Atmospheric Model," Proceedings of Euro-Par 2012 Workshops (HeteroPar), pp. 175--184, Rhodes Island, Greece, August 2012.

8. Akihiro Nomura, Yutaka Ishikawa, Naoya Maruyama, Satoshi Matsuoka, "Design and Implementation of Portable and Efficient Non-blocking Collective Communication," Proceedings of the 2012 IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid 2012), pp. 1--8, Ottawa, Canada, May 2012.

(3) Invited Talks

1. Naoya Maruyama, CUDA vs OpenACC: Evaluation of OpenACC Compilers with microbenchmarks and applications, Fourth symposium on Automatic Tuning Technology and its Application (4th ATTA), Invited talk, Dec 2012.

(4) Posters and presentations

1. Tetsuya Hoshino, Naoya Maruyama, Satoshi Matsuoka, "CUDA vs OpenACC: Performance Case Studies," GPU Technology Conference, Poster, San Jose, CA, USA, March 2013.

2. Keisuke Fukuda, Naoya Maruyama, Miquel Pericàs, Satoshi Matsuoka, "Fast Multipole Method on a Dynamic Scheduling Engine on Heterogeneous Environments," GPU Technology Conference, Poster, San Jose, CA, USA, March 2013.

3. Mohamed Wahib, Naoya Maruyama, "GPU-acceleration of a Weather Simulation Application: SCALE," GPU Technology Conference, Poster, San Jose, CA, USA, March 2013.

4. Tetsuya Hoshino, Naoya Maruyama, Satoshi Matsuoka, "Porting and Optimizing a Large-Scale CFD Application with CUDA and OpenACC," SIAM Conference on Computational Science and Engineering, MS162: Parallel Programming Models, Algorithms and Applications for Scalable Manycore Systems, Boston, USA, February 2013.

5. Naoya Maruyama, Satoshi Matsuoka, "Achieving High Performance and Portability in Stencil Computations," SIAM Conference on Computational Science and Engineering, MS162: Parallel Programming Models, Algorithms and Applications for Scalable Manycore Systems, Boston, USA, February 2013.

6. Miquel Pericas, Abdelhalim Amer, Keisuke Fukuda, Naoya Maruyama, Rio Yokota, Satoshi Matsuoka, "Towards a Dataflow FMM using the OmpSs Programming Model," IPSJ HPC, September 2012.

7. Motoshiko Matsuda, Naoya Maruyama, Implementing MapReduce on K-Computer, IPSJ SIG Notes HPC, July 2012.

8. Tetsuya Hoshino, Naoya Maruyama, Satoshi Matsuoka, Evaluation of Portability for a Real-world CFD Application with CUDA and OpenACC, IPSJ SIG Notes HPC, July 2012.

9. Kento Sato, Adam Mood, Kathryn Mohror, Todd Gamblin, Bronis R. De Supinski, Naoya Maruyama, Satoshi Matsuoka, "Design and Modeling of an Asynchronous Checkpointing System," IPSJ SIG-Notes HPC, July 2012.

10. Naoya Maruyama, "Physis: An Implicitly Parallel Framework for Stencil Computations," GPU Technology Confernence (GTC'12), San Jose, USA, May 2012.

(5) Patents and Deliverables
    -None

15. Advanced Visualization Research Team

15.1. Team members

Kenji Ono	(Team Leader)
Chongke Bi	(Postdoctoral Researcher)
Tomohiro Kawanabe	(Visiting Researcher)
Masahiro Fujita	(Visiting Researcher)
Kentaro Oku	(Visiting Researcher)
Hiroki Mizuno	(Visiting Researcher)
Yukiko Hayakawa	(Assistant)

15.2. Research Activities

The following is the objectives of our research in FY2012.

1) Installation of a cluster system for visualization and data processing research.

2) Development of a visualization software system for large-scale dataset.

3) Development of elemental techniques for visualization of large-scale dataset.

Researchers or engineers have their own scenarios for visualization and post processing. In addition, the well-known knowledge in each research field is utilized to comprehend phenomena and/or to lead scientific discovery. Many applications will help in the post processing process and it is efficient to apply the already existing software. However, all applications are not always operated on the K computer due to porting issue and so on. Our team has therefore introduced a widely used PC cluster system that has Intel CPU to offer the opportunity of running such applications. This cluster system will be directly connected to the global file system of the K computer in the next year. Moreover, the common visualization tools like VisIt, ParaView, and VMD will be installed on the visualization cluster.

On the other hand, application users strongly demand a visualization system that is able to operate on the K computer to avoid the extra copy of the dataset or to enhance the scalability of their applications. For this purpose, a visualization system named LSV has been now developing. The LSV system has been developed in the grand challenge program in RIKEN during 2007-2012, and its development is carried on into our team. The LSV system is originally designed for the commodity platforms such as Linux machine or clusters. This year, we investigated how to port the LSV system onto the K computer and found that the GLES/GLSL rendering API can be used instead of the conventional OpenGL API. We confirmed that a written test program worked well and could generate images on the K computer directly. The demonstration was conducted for molecular dynamics results.

Another point of view, it is of great significance to apply data compression method to the large-scale dataset generated from simulations. We have been investigating an efficient compression method

using proper orthogonal decomposition (POD) that enables us to reduce the data size small with high quality. Due to the limitation of memory size and computational cost, a parallel POD method has been proposed. A preliminarily test cases showed us that the proposed method have good potential but there is some room to improve the parallel efficiency.

Through the whole processes of computer simulation, it is important not only to manage the distributed files for high performance computation but also usability. To efficiently handle and manage the distributed file of Cartesian data structure, a lightweight file I/O library CIOlib was developed. This library provides functions; parallel distributed file I/O, management of distributed files, restart from different number of files N on M processes, restart with refinement, and restart with staging process on the K computer. This library will be applied for the simulation in the field of fluid, astrophysics and so on.

In SC12 conference, one of the AICS team gave a demonstration using Intel Phi processors, which showed a real-time climate CFD simulation including visualization. Our team took in charge of the visualization part. In this demonstration, the visualization was carried out by pre-computing and streaming technique, and showed reasonably fair frame rate.

So far, research activities in FY 2012 were summarized in above mentioned with three categories.

15.3. Research Results and Achievements

15.3.1. Installation of Visualization Cluster

Table 1 shows the specification of installed visualization cluster system and Fig. 1 depicts the structure of the system. Since this system is connected to the global file system of the K computer in original plan, no extra disk storage is supplied for this system now. There are two main purposes to operate this cluster. One is to run applications that are not able to operate on the K computer for some technical reasons, and the other is to offer an interactive visualization environment for users because the interactive environment for visualization is not offered yet. This cluster system will be operated for general post processing platform not only for visualization.

Table 1: Specification of visualization cluster.

Number of Node	Head node x 1 (Fujitsu PRIMERGY RX350 S7)
	Visualization node x 32 (Fujitsu PRIMERGY RX350 S7)
CPU	Intel Xeon E5-2670 x 2 (2.6GHz/8core)
Memory	64GB(8GBx8) >> 2TB(aggregate)
HDD	SAS 600GBx2(RAID1)
Network	InfiniBand QDRx1, LANx2
Operating System	Red Hat Enterprise Linux 6.1

In the next year, several extensions will be planned, such as the connection between this cluster and the global file system of the K computer, additional storage, and installation of GPUs.
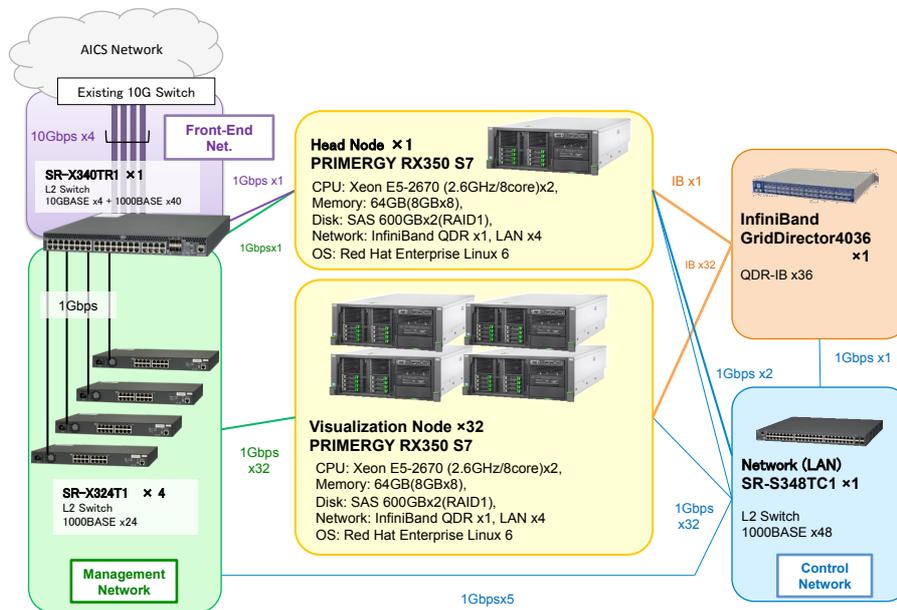
Figure 1: Configuration of an installed visualization cluster system.

15.3.2 Large-Scale Data Visualization System (LSV)

Fig.2 shows an internal logical design of the LSV system. The LSV system has a module structure and is designed so that the system can offer several useful visualization scenarios illustrated in Fig. 3. The LSV had been developed to operate on common PC clusters for these a couple of years. We had been discussed to make the LSV operate on the K computer. Usually, OpenGL API is used to render images but we found that OpenGL API is not supported on the K computer. We have decided to use OpenGL shading language (GLSL) for rendering API and OpenGL ES API (GLES) instead of the conventional OpenGL. A parallel ray-tracing program, which is a prototype of LSV's rendering kernel, was written by using GLES/GLSL and was compiled on the K computer. The parallel ray-tracer generated images as shown in Fig. 4 for the results of a molecular dynamics simulation and an extracted polygon data. Both images are rendered with the global illumination effect for better visibility. Fig. 5 also shows high quality and high resolution rendering image for the example polygon model. The global illumination and the ambient occlusion technique are used to increase visual quality.

15.3.3 Data Compression using Snapshot POD

Visualizing and analyzing large-scale dataset is an important task for scientific research in various fields. However, the visualization process is time-consuming, which is quite inconvenient for researchers and engineers to analyze the time-varying dataset. In order to resolve these problems, we proposed an approach to generate a small-scale dataset from the original large-scale one.
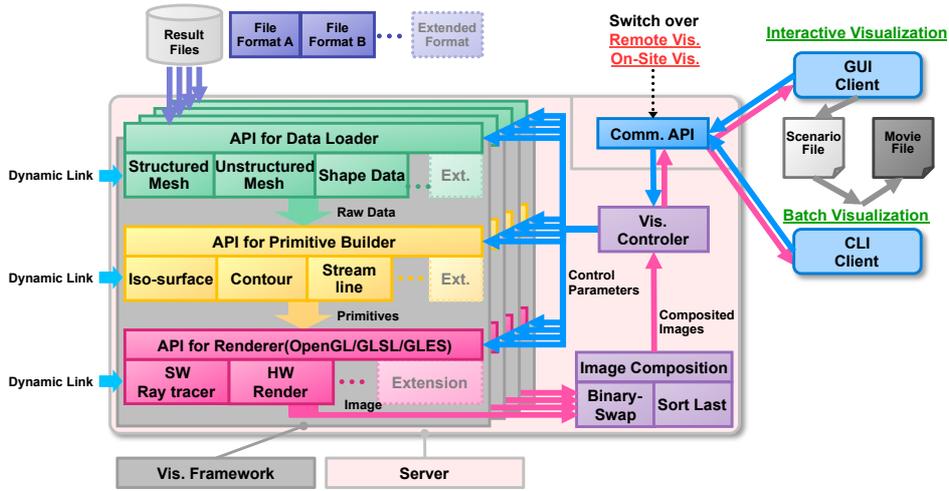
Figure 2: Logical design of a LSV system. Switching over the connection of modules, the LSV provides various operating scenarios for users.

Mode	Client	Vis. process
On-site	User PC	User PC
	Remote server	Server
Remote	User PC	Server

- **User interaction**
  - **Interactive** : **Images are generated by user's operation**
  - **Batch** : **Image/movie is obtained by predetermined scenario**

- **Timing**
  - **Real-time** : **InSitu**
  - **Post processing** : **File based method**

- **Renderer**
  - **Hardware** : **GPU rendering, high speed**
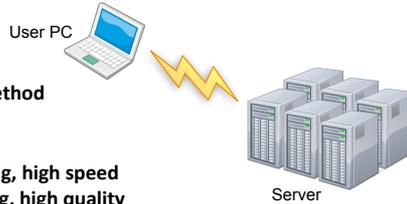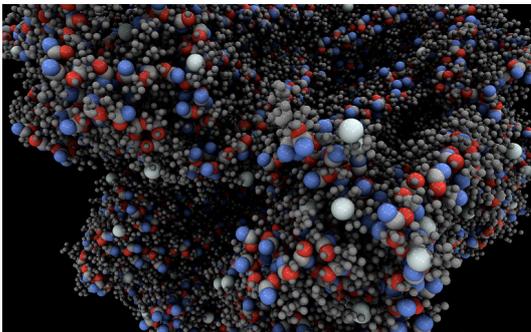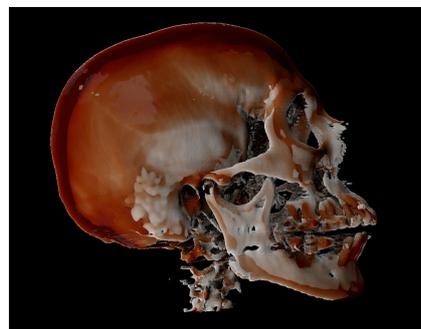 - **Software** : **CPU rendering, high quality**

Figure 3: User's operating scenario of visualization.

(a) PDB data

(b) Sub-surface scattering effect is applied for extracted iso-surface. Data is taken from Stanford CT Head data.

Figure 4: Parallel rendering results using GLSL API on the K computer.

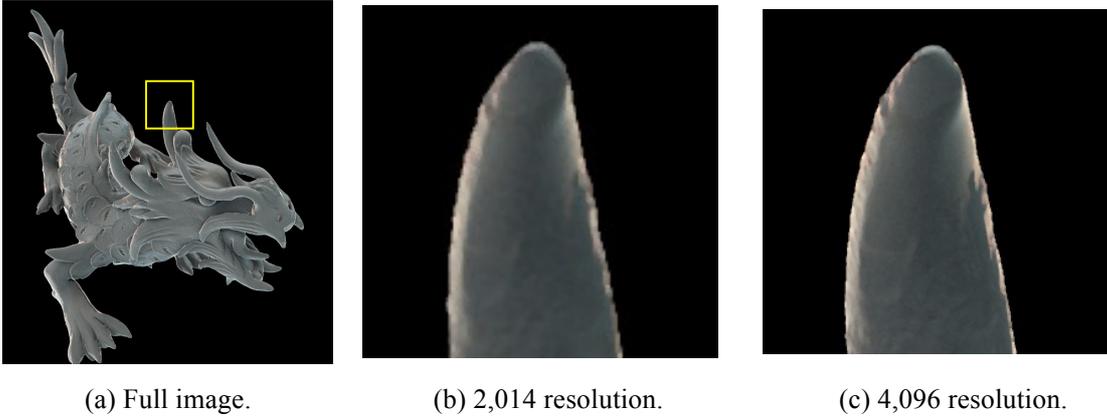(a) Full image.   (b) 2,014 resolution.   (c) 4,096 resolution.

Figure 5: A high-resolution image shows detail precisely. Figure (b) and (c) are closeup view of a yellow box in figure (a).

Figure 6 shows the detail of the proposed approach. The original dataset in the layer 0 was divided into 3 small groups firstly. POD algorithm is used to compress the datasets of the three small groups in parallel. However, if the compression process is stopped here, the compression ratio is 4/11, which is still high. Therefore the POD-basements in the layer 1 are compressed again as shown in the second line of Fig. 6. This process will be repeated until the POD-basements cannot be compressed any more. Restoring the compressed datasets efficiently is as important as compression process. In Fig. 6, the red arrows show the process of restoring the dataset in the 6th time step t_{0_6}. In the restoring process, it is unnecessary to calculate the POD-basements in the middle layers. The original datasets can be linearly restored using the POD-basements in the deepest layer and the related coefficients.
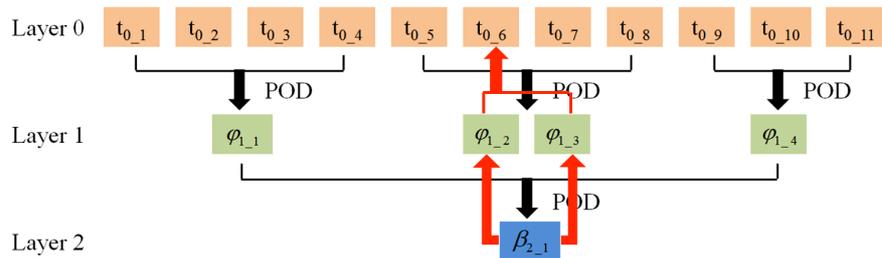
Figure 6: The flow chart of the proposed approach.

Figure 7 shows the result to compress a large-scale time-varying dataset ($500 \times 200 \times 125 \times 139$ [$x \times y \times z \times$timesteps]) obtained from a flow simulation in the air jet mixer of a machinery, which is rendered by the magnitude of velocity (Fig. 7(a)). The colors of red, green, magenta, and blue represent original dataset, the compression results with 6 nodes, 7 nodes, and 8 nodes in parallel, respectively. Fig. 7(b) is the compression ratio calculated. The result shows that our approach can

successfully compress such kind of large-scale dataset in a quite low compression ratio. Meanwhile, the precision of the compressed dataset can also be preserved in such low compression ratio, as shown in Fig. 7(c). Here, the number of parabola shape is the same with the numbers of nodes. These parabola shapes can be used to prove the correctness of our algorithm. This is because the mean velocity for the neighbor time steps is nearly equal to that of the middle time step in a small size group. Furthermore, the computational cost is also investigated in temporal space, as shown in Fig. 7(d). It becomes smaller as the numbers of parallel nodes are increased. This also described one of the merits of our parallel algorithm.
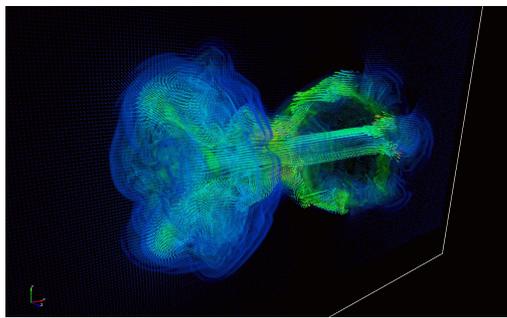
(a) Flow field of sample data. Color means the magnitude of velocity.
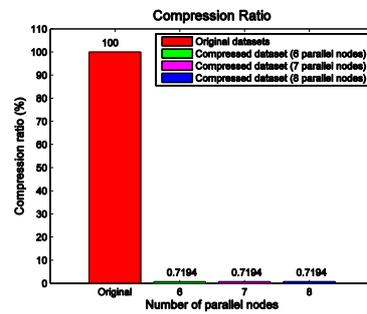
(b) Compression ratio for different parallel cases.
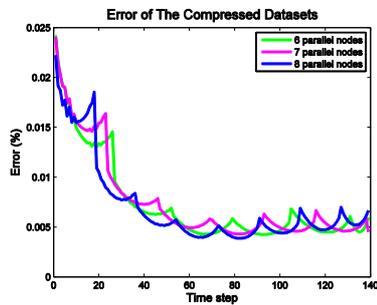
(c) Error distribution.
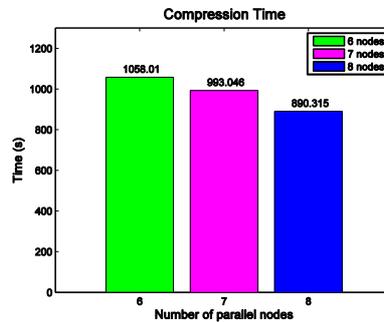
(d) Comparison of compression time for different parallel cases.

Figure 7: Result of compressed a large-scale dataset of a flow simulation in the air jet mixer.

15.4. Schedule and Future Plan

In addition to the three topics listed in section 2, several elemental technologies, e.g., knowledge extraction by agent-based method, in-situ visualization, tiled-display technology and parallel particle tracking, will be investigated in the next year.

15.5. Publication, Presentation and Deliverables

(1) Journal Papers

1. Bi, C., Sakurai, D., Takahashi, S. and Ono, K.: Interactive Control of Mesh Topology in

Quadrilateral Mesh Generation Based on 2D Tensor Fields, Lecture Notes in Computer Science, Advances in Visual Computing, Vol. 7432, pp. 726-735, (2012).

2. Ono, K., Advanced Visualization Technology on Large-Scale Numerical Simulation, Journal of the Visualization Society of Japan, Vol, 32, No.125, pp.1-6, (2012).

(2) Conference Papers

1. Ono, K., Kawanabe, T. and Hatada, T.: HPC/PF - High Performance Computing Platform: An Environment that Accelerates Large-Scale Simulations, Vecpar 2012, (2012).

2. Mao, X., Watanabe, D. and Ono, K.: Gaze-Directed Flow Visualization, Proceedings of the Conference on Computational Engineering and Science, Vol.17, (2012).

3. Suzuki, S. and Ono, K.: An Efficient Data Structure of Building-Cube Method for Large-Scale Computation, Proceedings of the Conference on Computational Engineering and Science, Vol.17, (2012).

4. Ono, K., Mizuno, H., Mukai, Y. and Oku, K.: Development of technology for very-large-scale voxel generation and its interface for simulators, Proceedings of the Conference on Computational Engineering and Science, Vol.17, (2012).

5. Suzuki, S., Ono, K., Ogawa, T. and Onishi, J.: A Software Framework of the Building-Cube Method for a Large-scale Computation, MASCOT and ISGG 2012, (2012).

6. Onishi, J. and Ono, K.: Development of a parallel Poisson equation solver for two-phase flow simulations, MASCOT and ISGG 2012, (2012).

7. Ono, K.: Technology that joins product design and simulation‑ Construction of HPC/PF and its application scenario, JSME 25th Computational Mechanics Division Conference, (2012).

8. Onishi, J. and Ono, K.: Convergence properties of the Poisson equation solvers for two-phase fluid flows (2nd report: Applicability of the MultiGrid Preconditioned Conjugate Gradient Method), The 26th CFD symposium, B09-4, (2012).

9. Onishi, J. and Ono, K.: Verification of a sharp interface method for two-phase flow simulations, Annual meeting of The Japanese Society for Multiphase Flow 2012, (2012).

(3) Invited Talks

1. Ono, K.: Strategy of Visualization toward Exa-Scale Computing, PC cluster consortium workshop in Kyoto, Jan., Kyoto, Japan, (2012).

2. Ono, K.: Automatic Grid Generation over 10 Billion Scale and Visualization, VINAS user group meeting, Oct., Tokyo, Japan, (2012).

3. Ono, K., Onishi, J. and Kawanabe, T.: Issues and approach for large-scale CFD on K computer, International Workshop on Future of CFD and Aerospace Sciences, Dec., Pusan, Korea, (2012).

(4) Posters and presentations

1. Ono, K.: Large-scale CFD for Industrial Application and Post Processing, 3rd International WS of large-scale visualization, Oct., Kobe, Japan, (2012).

2. Ono, K.: Research Activities of Visualization on K-computer, The 3rd AICS International Symposium: Computer and Computational Science for Exascale Computing, Feb., Kobe, Japan, (2013).

3. Ono, K.: Role of numerical library on road map for exa-flops computer, Automatic Tuning Research Group meeting, Jul., Koganei, Tokyo, (2012).

4. Bi, C. and Ono, K.: POD-Based Parallel Compression for Visualizing Large-Scale Dataset, High Performance Computing Symposium 2013, Jan., Tokyo, Japan, (2013).

(5) Patents and Deliverables
      -None

16. Data Assimilation Research Team

16.1. Team members

Takemasa Miyoshi (Team Leader)

Shigenori Otsuka (Postdoctoral Researcher)

Juan J. Ruiz (Visiting Researcher)

Keiichi Kondo (Student Trainee)

Yukiko Hayakawa (Assistant)

16.2. Research Activities

Data Assimilation Research Team (DA Team) was launched on 1 October 2012 and is composed of four research staff as of March 2013. Data assimilation is a cross-disciplinary science to synergize numerical simulations and observational data, using statistical methods and applied mathematics. As computers become more powerful and enable more precise simulations, it will become more important to compare the simulation with actual observations. DA Team performs cutting-edge research and development on advanced data assimilation methods and their wide applications, aiming at integrating computer simulations and observational data in the wisest way. Particularly, DA Team will tackle challenging problems of developing efficient and accurate data assimilation systems for high-dimensional simulations with large amount of data. The specific areas include 1) research on parallel-efficient algorithms for data assimilation with the super-parallel K computer, 2) research on data assimilation methods and applications by taking advantage of the world-leading K computer, and 3) development of most advanced data assimilation software optimized for the K computer.

In FY2012, we focused on 1) theoretical research on challenging problems in data assimilation, and 2) cutting-edge data assimilation research on meteorological applications. We have made substantial progress as follows:

1. An objective approach to model parameter estimation using data assimilation was investigated. (1 paper accepted)
2. Theories on discrete filtering to deal with model imperfections in ensemble-based data assimilation were explored.
3. A new approach to multi-scale covariance localization was invented and investigated.
4. The Local Ensemble Transform Kalman Filter (LETKF) system with a mesoscale numerical weather prediction model known as the Weather Research and Forecasting (WRF) model was ported to the K computer.

Main achievements are highlighted in the next section.

16.3. Research Results and Achievements

16.3.1. Model parameter estimation

In general, numerical simulation models contain a number of tuning parameters, and usually they are optimized manually and subjectively. Efforts have been made to make the tuning process objective and automatic, so that we find optimal parameters and make the simulation fit better to the observations. We have explored an approach to analyzing an augmented state vector consisting of both prognostic variables and model parameters through ensemble-based data assimilation. This allows estimating both prognostic state variables and model parameters simultaneously through data assimilation. Ruiz et al. (2013) explored the approach with an intermediate atmospheric general circulation model known as the SPEEDY model. Figure 1 shows the time series of three convective parameterization model parameters. Bad initial values converge to the right values (dashed lines) shortly after data assimilation both for temporally-fixed parameters (left panel) and for temporally-varying parameters (right panel).
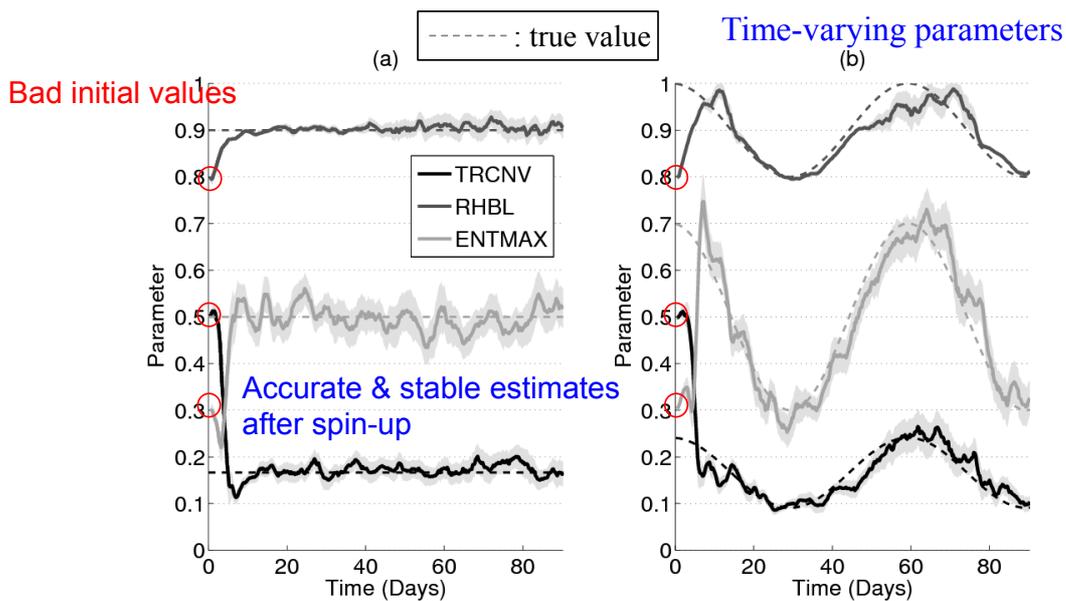
Fig. 1.

With the success from the idealized experiments with the SPEEDY model, we applied this approach to a real Typhoon case in 2008. Using the WRF-LETKF system (Miyoshi and Kunii 2012), air-sea exchange coefficients are estimated as a two-dimensional field. Figure 2 indicates estimated moisture exchange coefficients. The value 1 is the default; 1.5 and 0.5 correspond to 50% more and less effective air-sea exchange of the moisture fluxes, respectively. Over the Pacific, the estimated parameters suggest reducing moisture fluxes from the sea surface. As a result, biases are reduced,

and Typhoon Sinlaku's forecast was improved.

MOISTURE FLUX CORRECTION FACTOR
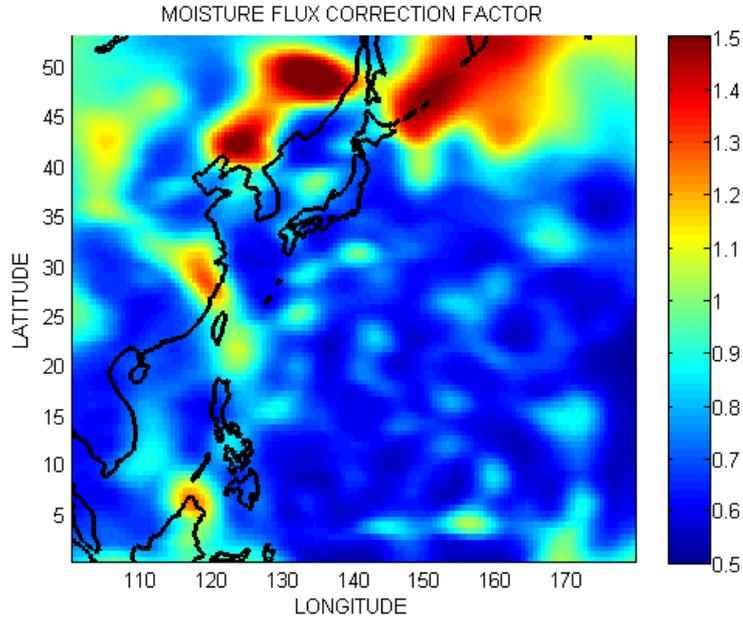
Fig. 2.

16.3.2 Theoretical development on multi-scale covariance localization

Ensemble-based data assimilation methods have been improved consistently and have become a viable choice in operational numerical weather prediction. A number of issues for further improvements have been explored, including flow-adaptive covariance localization and advanced covariance inflation methods. Dealing with multi-scale error covariance and model errors is among the unresolved issues that would play essential roles in analysis performance. With higher resolution models, generally narrower localization is required to reduce sampling errors in ensemble-based covariance between distant locations. However, such narrow localization limits the use of observations that would have larger-scale information. Previous attempts include successive covariance localization by F. Zhang et al. who proposed applying different localization scales to different subsets of observations. The method aims at using sparse radiosonde observations at a larger scale, while using dense Doppler radar observations at a small scale simultaneously. This study aims at separating scales of the analysis increments, independent of observing systems. Inspired by M. Buehner, we applied two different localization scales to find analysis increments at the two separate scales, and obtained astonishing improvements at all scales in simulation experiments using the SPEEDY model.

Figure 3 illustrates analysis increments from a single station observation at the star point. δx_h on the top right indicates the analysis increment from the raw ensemble perturbations with a

narrower 500-km localization scale. This shows a small-scale feature near the observed location. δx_l on the bottom right indicates the analysis increment from a smoothed ensemble perturbations with a wider 1000-km localization scale. This shows smoother structure in the longer distance, although lacks structure in the shorter range. Merging δx_h and δx_l, although not the simple sum, gives the left panel, in which both smaller-scale structure in the shorter range and smoother structure in the longer range are preserved. With this new multi-scale localization method, we obtained large improvement mostly in the moisture and precipitation analyses.
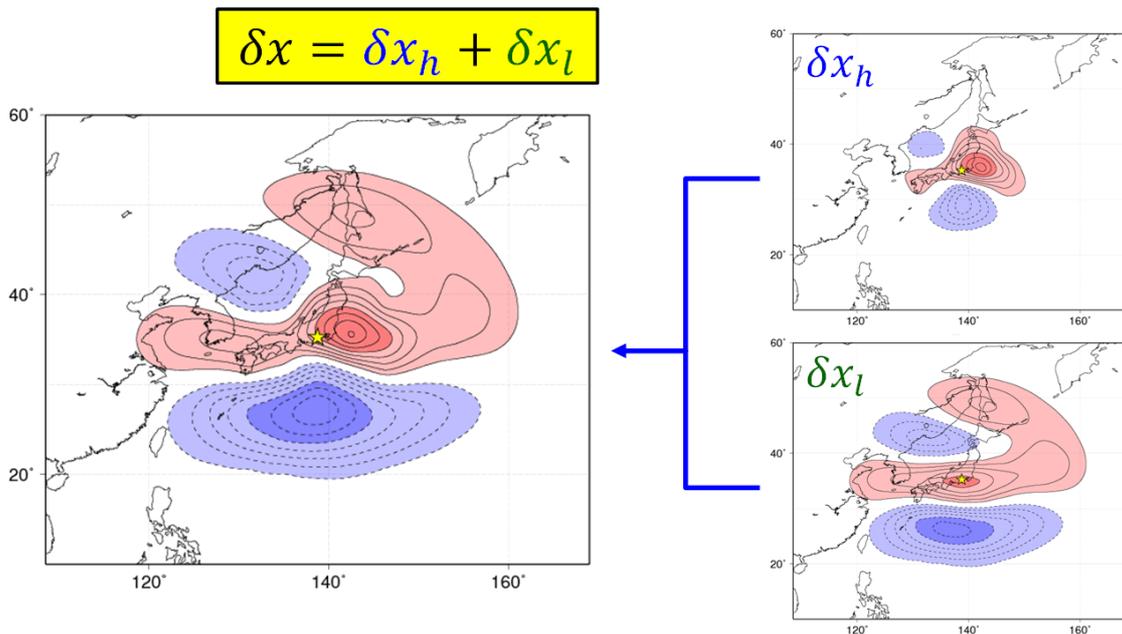
Fig. 3.

16.3.3 Porting the WRF-LETKF system to the K computer

For leading meteorological research using the K computer and for improving the computational efficiency of the widely-used LETKF code, we use the WRF-LETKF system (Miyoshi and Kunii 2012) as a testbed. SPIRE (Strategic Programs for Innovative Research) Field 3 performs research on super-high-resolution mesoscale numerical weather prediction using the LETKF, and DA Team aims at aiding their research through close collaboration on this LETKF code. As the first step, we ported the WRF-LETKF system on the K computer, and measured the current computational performance. Table 1 shows the computational time for a single-member, 6-hour WRF forecast for the default 60-km WRF-LETKF system, and its higher-resolution 20- and 5-km versions. Table 2 shows a similar table for the LETKF computations. These two tables suggest that the parallel efficiency is about 10% of the optimal for the 5-km experiment compared with the 60-km experiment. Our future work includes optimizing the parallel efficiency for the K computer,

especially with larger ensemble sizes.

To confirm that the LETKF works properly on the K computer, 6-hour forecast fields from the LETKF analyses were investigated. Figure 4 shows 6-hour accumulated rain (shading, mm/6h) and mean-sea-level pressure (contours) for a low pressure system on 9 August 2008, after about a week spin-up of the LETKF data assimilation. The low pressure system is analyzed reasonably well for the three experiments at different resolutions. It is apparent that the 5-km experiment produces very fine structure of the rain bands associated with the low.

Table 1. Timing for the WRF forecasts.

Resolution	Number of nodes (CPU)	Max memory per node	Wall time (sec.)
60 km	13 (104)	0.914 GB	107
20 km	15 (120)	1.4 GB	452
5 km	50 (400)	6.3 GB	6320

Table 2. Timing for the LETKF analysis.

Resolution	Number of nodes (CPU)	Max memory per node	Wall time (sec.)
60 km	10 (80)	3.2 GB	130
20 km	40 (320)	4.4 GB	440
5 km	500 (4000)	8.4 GB	3000
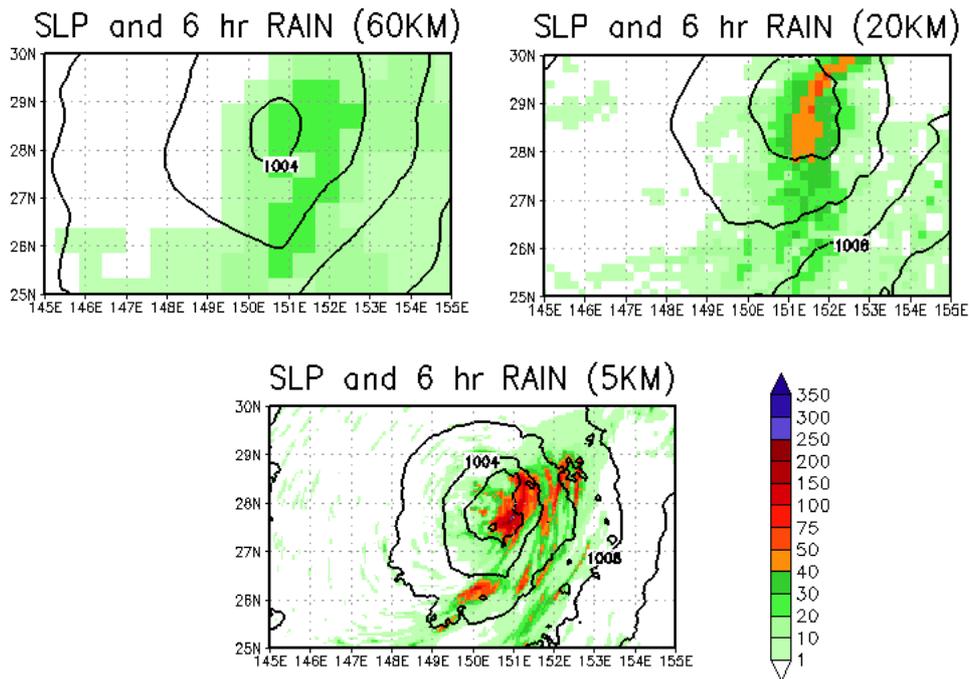
Fig. 4.

16.4. Schedule and Future Plan

Based on the achievements in FY2012, it is apparent that we need to optimize the LETKF code for the K computer, particularly for massively parallel computations. The current WRF-LETKF system does not perform well enough with the K computer, and algorithmic development will be necessary. Also, we will keep working on the fundamental theoretical problems of multi-scale and model-error treatments and of model parameter estimation. Besides, we will explore more theoretical aspects including non-linear and non-Gaussian treatments. These theoretical studies will improve the capability of ensemble-based data assimilation in wide applications. Moreover, we plan on seeking wider applications of data assimilation beyond geophysical applications. We will start working on exploratory investigations in FY2013.

16.5. Publication, Presentation and Deliverables

(1)   Journal Papers

1.   Greybush, S. J., R. J. Wilson, R. N. Hoffman, M. J. Hoffman, **T. Miyoshi**, K. Ide, T. McConnochie, and E. Kalnay, 2012: Ensemble Kalman Filter Data Assimilation of Thermal Emission Spectrometer (TES) Temperature Retrievals into a Mars GCM. *J. Geophys. Res.*, **117**, E11008. doi:10.1029/2012JE004097

2.   Hoffman, M. J., **T. Miyoshi**, T. Haine, K. Ide, C. W. Brown, and R. Murtugudde, 2012: An Advanced Data Assimilation System for the Chesapeake Bay: Performance Evaluation. *J.*

Atmos. Oceanic Tech., **29**, 1542-1557. doi:10.1175/JTECH-D-11-00126.1

3. Kunii, M. and **T. Miyoshi**, 2012: Including uncertainties of sea surface temperature in an ensemble Kalman filter: a case study of Typhoon Sinlaku (2008). *Weather and Forecasting*, **27**, 1586-1597. doi:10.1175/WAF-D-11-00136.1

4. Kang, J.-S., E. Kalnay, **T. Miyoshi**, J. Liu, and I. Fung, 2012: Estimation of surface carbon fluxes with an advanced data assimilation methodology. *J. Geophys. Res.*, **117**, D24101. doi:10.1029/2012JD018259

5. **Miyoshi, T.**, E. Kalnay, and H. Li, 2013: Estimating and including observation error correlations in data assimilation. *Inverse Problems in Science and Engineering*, **21**, 387-398. doi:10.1080/17415977.2012.712527

6. **Otsuka, S.**, S. Nishizawa, T. Horinouchi, and S. Yoden, 2013: An experimental data handling system for ensemble numerical weather predictions using a web-based data server and analysis tool "Gfdnavi". *J. Disaster Research*, **8**, 48-56.

7. **Ruiz, J. J.**, M. Pulido, and **T. Miyoshi**, 2013: Estimating model parameters with ensemble-based data assimilation: A review. *J. Meteorol. Soc. Japan*, **91**, in press. doi:10.2151/jmsj.2013-201

(2) Conference Papers
    -None

(3) Invited Talks

1. **March 2013** Takemasa Miyoshi, "Challenges of Ensemble-based Data Assimilation for Large-Scale Simulations", Invited Presentation, The 3rd AICS International Symposium, RIKEN/AICS, Kobe, Japan.

2. **January 2013** Takemasa Miyoshi, "Advances and Challenges in Ensemble-based Data Assimilation in Meteorology", Invited Presentation, Third Data Assimilation Workshop, Institute of Statistical Mathematics, Tachikawa, Tokyo, Japan.

3. **October 2012** Takemasa Miyoshi, "Observation Impact Estimates with an Ensemble-based Approach", Invited Presentation, International Symposium on Data Assimilation, German Weather Service (DWD), Offenbach, Germany.

4. **October 2012** Juan Ruiz, "Data Assimilation-based parameter estimation schemes", Exploring the Use of Data Assimilation Methods for the Detection and Attribution of Climate Change, Buenos Aires, Argentina.

5. **November 2012** Juan Ruiz, "Estimating model error with the ensemble Kalman filter", Invited Presentation, WCRP-SPARC Workshop, Buenos Aires, Argentina.

(4)   Posters and presentations

1. **Miyoshi, T.***, **K. Kondo**, S.-C. Yang, and E. Kalnay: Spatial Structure of the LETKF Weights and Multi-scale Treatment in an EnKF. American Meteorological Society Annual Meeting, Austin, TX, USA, January 8, 2013.

2. **Ruiz, J. J.**, **T. Miyoshi***, M. Kunii, and M. Pulido: Self-optimization of Model Parameters with the LETKF: from Idealized Experiments to a Real-world Application. American Meteorological Society Annual Meeting, Austin, TX, USA, January 8, 2013.

3. **Miyoshi, T.*** and **K. Kondo**: Multi-scale Treatment in Ensemble Data Assimilation. Meteorological Research Institute, Tsukuba, Japan, February 13, 2013.

4. **Miyoshi, T.*** and **K. Kondo**: An approach to multi-scale localization. Nichii-gakkan, Kobe, Japan, March 21, 2013.

5. **Kondo, K.***, **T. Miyoshi**, and H. L. Tanaka: Multiscale localization in ensemble-based data assimilation. AICS International Workshop on Data Assimilation, RIKEN/AICS, Kobe, Japan, February 26-27, 2013.

6. **Ruiz, J. J.***, **T. Miyoshi**, and M. Kunii. Self-optimization of Model Parameters with the LETKF: a Real-world Application. AICS International Workshop on Data Assimilation, RIKEN/AICS, Kobe, Japan, February 26-27, 2013.

7. **Otsuka, S.***, N. J. Trilaksono, and S. Yoden: Statistics on Convections during the Jakarta Flood Event in 2007 Simulated by JMA-NHM. The 3rd AICS International Symposium, RIKEN/AICS, Kobe, Japan, February 28-March 1, 2013.

(5)   Patents and Deliverables

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

17. Computational Chemistry Research Unit

17.1. Unit members

Kimihiko Hirao (Unit Leader)

Jong-Won Song (Research Scientist)

Rahul Kar (Postdoctoral Researcher)

Takao Tsuneda (Senior Visiting Scientist)

17.2. Research Activities

There are two major approaches in investigating the electronic structure theories of molecules: wavefunction methods and density functional theory (DFT). For more than 30 years, huge amount of efforts have been made to enhance wavefunction methods to become well-accepted state-of-the-art methodologies. Using the wavefunction methods, accurate results can be obtained for small systems. However, it is rather difficult to handle very large systems due to the steep N-dependence. Instead of the wavefunction methods, DFT has emerged as a powerful computational tool to study chemical systems for its simplicity, concept, and applicability to large systems. However, DFT has not reached such a mature stage as wave function methods.

One large drawback of DFT is that there is no means of systematically improving DFT energies. The accuracy is dictated by the exchange-correlation functional employed. DFT also fails to describe induced/response properties. The failures mainly arise from the wrong long-range behavior due to the local character of the approximate exchange-correlation functionals. So far, we have developed long-range corrected density functional theory (LC-DFT) to solve many problems found in conventional DFT. The development of LC-DFT had a large impact in theoretical chemistry and the number of research based on LC-DFT is growing intensively.

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

17.3. Research Results and Achievements

17.3.1. Long-range Corrected Functionals Satisfy Koopmans' Theorem

Recently, we found a new feature of long-range corrected density functional theory (LC-DFT): LC-DFT is the first and only method to give valence orbital energies quantitatively. Molecular orbitals provide us insights to clarify chemical processes as seen in frontier molecular orbital theory.

However, orbital energies have not been emphasized in investigating chemical processes, because there has never been a method that can quantitatively obtain orbital energies. LC-DFT is now going to change this situation.

In this project, we have shown that long-range corrected density functionals reproduce highly-accurate valence orbital energies beyond comparison to those of other methods. Figure 1 illustrates the HOMO-LUMO gaps of LC-DFT compared to the vertical electron affinities (EAs) minus vertical ionization potentials (IPs) that are calculated by CCSD(T)/6-311++G(3df,3pd) for 113 molecules. We found that molecular orbitals obtained by LC functionals almost meet the Koopmans' theorem, which establishes that HOMO and LUMO energies are identical to the minus corresponding IP and EA, respectively. We also showed that the valence orbital energies and HOMO-LUMO gaps of LC functionals are better than those of recently proposed ωM05-D [*J. Chem. Phys.* **136**, 154109 (2012)]. We have also decomposed the IP energies into the orbital, relaxation, and correlation energies. It is found that the LC-DFT inherently includes more relaxation effects than the Hartree-Fock method does and contains more correlation effects than conventional density functionals do.
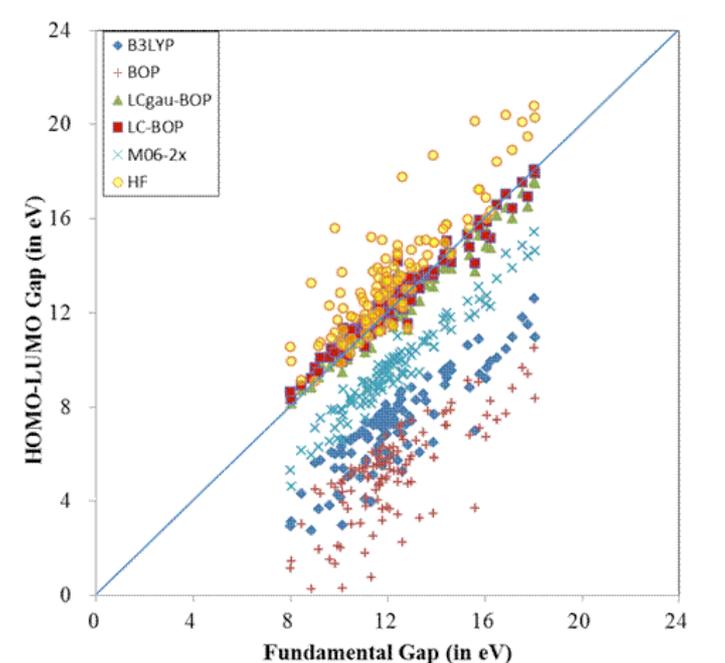
Fig. 1. Calculated HOMO-LUMO energy gap versus reference fundamental gap for 113 molecules. Reference fundamental gap are calculated using IP and EA calculated by CCSD(T). (Taken from R. Kar, J.-W. Song, K. Hirao, J. Comput. Chem., 34, 958–964 (2013))

17.3.2. Improvement of LC-DFT functional performance on thermochemical properties

Various exchange and correlation functionals have been developed to enhance the applicabilities of DFT. One-parameter progressive (OP) correlation functional that we have previously developed is

a flexible correlation functional, which progressively depends on the exchange functional employed. In our previous study, long-range corrected exchange functionals and its Gaussian-attenuated functionals (LCgau) have been combined with the OP correlation functional. However, the parameter in the OP functional has not been optimized taking the exchange potential into account. We therefore examined to re-optimize the parameter.

The parameter of the OP correlation functional was optimized combining with the LC- and LCgau-applied Becke88 exchange functionals for atomization energies. As a result, we confirmed that the LC-BOP and LCgau-BOP functionals with the new parameter perform well in calculations of several properties compared to our previous calculations as shown in Fig. 2.
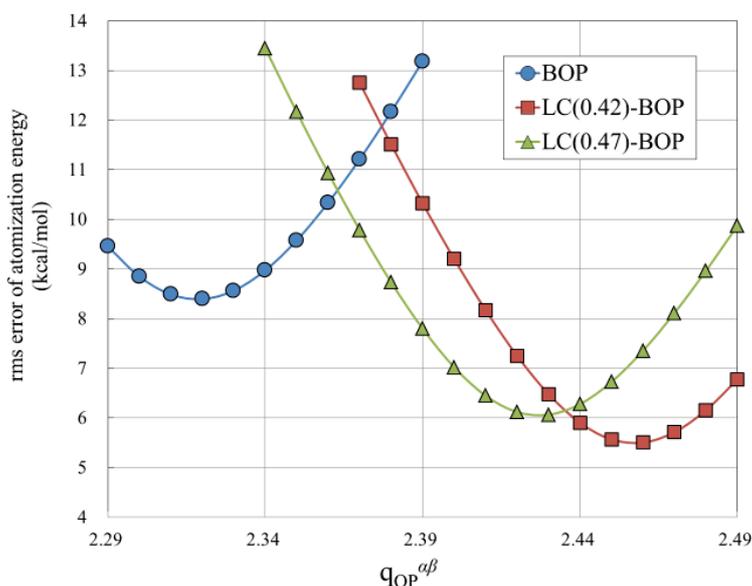
Fig. 2. The root mean square (rms) error of the G2 set atomization energies (148 molecules) depending on the μ parameter of the BOP functional and the LC-BOP functional with $\mu = 0.42$ and 0.47. (Taken from J.-W. Song, K. Hirao, Chem. Phys. Lett., 563, 15–19 (2013)).

17.3.3. The development of DFT functional applicable to solid states

To predict accurate band gaps by orbital energy gaps has been of substantial importance in developing new materials. However, conventional DFT functionals have been reported to give orbital energy gaps smaller than experimental band gaps for semi-conductors used in e.g. solar cells. Although several hybrid functionals such as Heyd-Scuseria-Ernzerhof (HSE) have been developed to make orbital energy gaps of semi-conductors close to band gaps, the computational cost of calculations using HSE is too demanding.

Recently, we developed a new functional for solid state band gap calculations, which is called Gau-PBE hybrid functional, that uses a Gaussian function as a modified Coulomb operator and is applied to Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional. In the Gaussian-basis

calculations, the new functional is found to give much more accurate band gaps, described as orbital energy gaps, than those of HSE with much less computational time as shown in Fig. 3.

Moreover, we implemented our Gau-PBE functional in a periodic quantum chemistry software, Quantum ESPRESSO. It is well known that, in periodic calculations, hybrid functionals obtain orbital energy gaps close to the band gaps, but is too much time consuming. The new functional has no singularity problem in the Fock matrix calculations that is usually given in hybrid functional calculations. As a result, we confirmed that our new implemented functional as the most computational time saving method.

We also updated the Gau-PBE functional by adopting the Ernzerhof-Perdew exchange hole (EP) model to the DFT exchange part of PBE. The new functional is named Gau-PBEh. Applying the EP model to the DFT part of Gau scheme contributes to the improvement of the performance over atomization energies and solid state lattice constants. In addition, Gau-PBEh takes nearly the same computation time for band gap calculations as Gau-PBE, implying that less than 60% of the time taken in HSE hybrid DFT functional calculations.
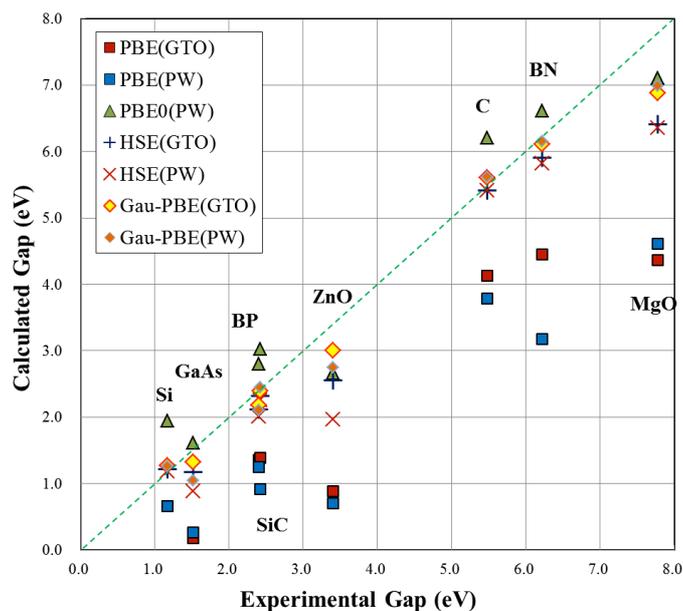
Fig. 3. A comparison of band gaps calculated using PBE, PBE0, HSE, and Gau-PBE vs experimental band gaps. The band gaps using both Gaussian-type-orbital and plane waves are presented. In plane wave calculations, 24×24×24k/6×6×6q is used. Only in ZnO, 8×8×8k/4×4×4q is used. (Taken from J.-W. Song, K. Yamashita, K. Hirao, J. Chem. Phys. 137, 244105 (2012))

17.3.4. LC-DFT application to Diels-Alder reactions

Diels-Alder reactions have been important target systems in quantum chemistry especially for chemical reactivity calculations. The empirical frontier molecular orbital theory has been used to interpret or to predict both the reaction rates and regioselectivities of the Diels–Alder reactions by

frontier (HOMO and LUMO) orbitals. The reactivities of the Diels–Alder reactions have been analyzed with global hardness, usually approximated as a half of the HOMO-LUMO gap. Recently, we found that LC-DFT reproduces HOMO-LUMO gap quantitatively. In this study, we seek the possibility of quantitative reaction analysis on the orbital energies of LC-DFT.

First, we calculated the Diels–Alder reaction enthalpies that have been poorly given by conventional functionals including B3LYP functional. As a result, it is found that the long-range correction drastically improves the reaction enthalpies. The barrier height energies were also computed for these reactions. Consequently, we found that dispersion correlation correction is also crucial to give accurate barrier height energies. It is, therefore, concluded that both long-range exchange interactions and dispersion correlations are essentially required in conventional functionals to investigate Diels–Alder reactions quantitatively. After confirming that LC-DFT accurately reproduces the orbital energies of the reactant and product molecules of the Diels–Alder reactions, the global hardness responses, the halves of HOMO-LUMO energy gaps, along the intrinsic reaction coordinates of two Diels–Alder reactions were computed as shown in Figure 4. We noticed that LC-DFT results satisfy the maximum hardness rule for overall reaction paths while conventional functionals violate this rule on the reaction pathways. Furthermore, our results also show that the HOMO-LUMO gap variations are close to the reaction enthalpies for these Diels–Alder reactions. Based on these results, we foresee quantitative reaction analysis on the orbital energies.
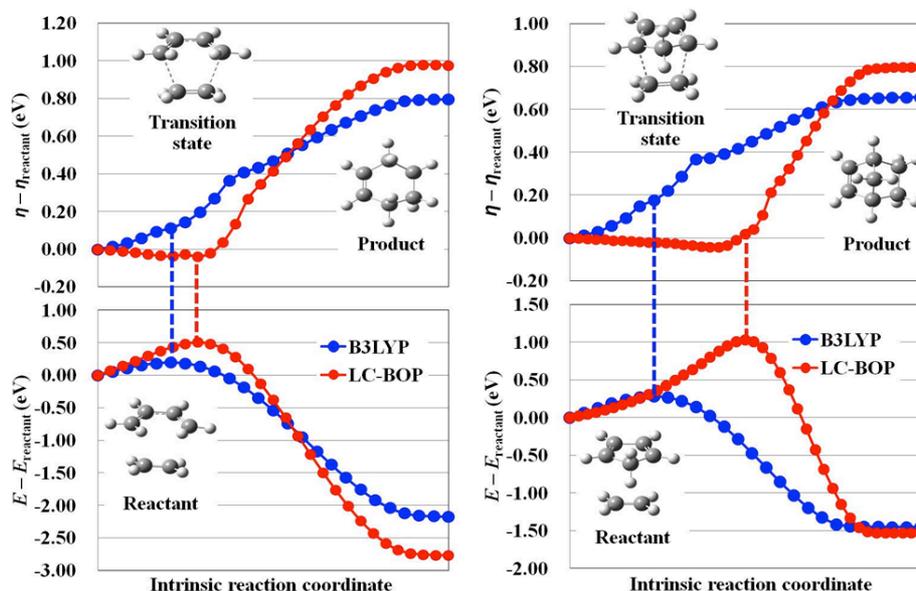

Fig. 4. Global hardness responses and total energies along the intrinsic reaction coordinates for the reactions of butadiene with ethylene a) and cyclopentadiene with ethylene b). Global hardness responses and total energies are set to be zero at the reactants. (Taken from R. K. Singh, T. Tsuneda, J. Comput. Chem. 34, 379−386 (2013))

17.4. Schedule and Future Plan

In the next fiscal year, we perform the following studies to expand the applicabilities of LC-DFT.

First, we are developing the order-N calculation algorithm of LC-DFT to calculate large molecular systems quantitatively with much less computational time. We will then apply this algorithm to excited state calculations on time-dependent density functional theory (TDDFT). We will also develop open-shell spin-orbit TDDFT to calculate molecular systems including metal atoms. Furthermore, we will carry out nonadiabatic coupling calculations based on TDDFT to reproduce photochemical reactions comprehensively. We are also planning to apply Gau-PBE and Gau-PBEh methods to solid state calculations of real systems.

17.5. Publication, Presentation and Deliverables

(1) Journal Papers

1. J.-W. Song, K. Yamashita, K. Hirao, "Gaussian attenuation hybrid scheme applied to Ernzerhof-Perdew exchange hole model (Gau-PBEh)", J. Chem. Phys. 137, 244105 (2012).

2. K. Hirao, "The K Computer: User-Friendly", Science 338, 1149–1149 (2012).

3. K. Hirao, "Special Contribution Japan's K Computer Project", FUJITSU Sci. Tech. J. 48, 247–254 (2012).

4. R. Kar, J.-W. Song, K. Hirao, "Long-Range Corrected Functionals Satisfy Koopmans' Theorem: Calculation of Correlation and Relaxation Energies", J. Comput. Chem., 34, 958–964 (2013).

5. R. K. Singh, T. Tsuneda, "Reaction Energetics on Long-Range Corrected Density Functional Theory: Diels-Alder Reactions", J. Comput. Chem. 34, 379–386 (2013).

6. J.-W. Song, K. Hirao, "Long-range corrected density functional theory with optimized one-parameter progressive correlation functional (LC-BOP12 and LCgau-BOP12)", Chem. Phys. Lett., 563, 15–19 (2013).

(2) Review Articles and Books

1. T. Tsuneda, "Fundamentals of Density Functional Theory", (Kodansha) (2013). (in Japanese).

2. T. Tsuneda, "π-Stacking on Density Funtional Theory: A Review", in π-Stacked Polymers and Molecules, edited by T. Nakano (Springer-Verlag) (2013).

(3) Invited Talks

1. K. Hirao, "Recent Advances in LC-DFT", "Electronic Structure Theory for Strongly Correlated Systems", Hotel La Torre, Palermo, Italy, May 30– Jun. 1 (2012).

2. K. Hirao, "Long-Range Corrected DFT Functional", University of Delaware, Newark, USA, Aug. 1–3 (2012).

3. T. Tsuneda, "Density Functional Theory for Chemistry", 52nd Summer School of Young Molecular Scientists' Association, University of Tokyo, Tokyo, Japan, Aug. 20–24 (2012). (In Japanese)

4. K. Hirao, "The K Computer and Science", Theory and Applications of Computational Chemistry (TACC2012), Pavia, Italy, Sep. 2–7(2012).

5. T. Tsuneda, "History and Recent Progress in Research on Orbital Energies", 24th Quantum Chemistry Seminar, Waseda University, Tokyo, Japan, Jan. 17 (2012). (In Japanese)

6. T. Tsuneda, "New Findings in Research on Orbital Energies", Supercomputer Workshop, Okazaki Conference Center, Okazaki, Japan, Jan. 22–23 (2013). (In Japanese)

7. K. Hirao, "Long-Range Corrected DFT Functionals", CRC International Symposium in Strasbourg "Chemical Theory for Complex Systems", University of Strasbourg, Strasbourg, France, Mar. 7–8 (2013).

8. T. Tsuneda, "Necessity of Long Range Correction in DFT for Dispersion Interaction Calculation", The 68th Annual Meeting of the Physical Society of Japan (Symposium), Hiroshima University, Higashi-Hiroshima, Japan, Mar. 26–29 (2012). (in Japanese)

(4) Posters and presentations

1. J.-W. Song, K. Hirao, "Which is Better: An Error Function or Gaussian Attenuation in Hybrid Density Functional Theory for Solid State Calculations?", The 14th International Congress of Quantum Chemistry, Boulder, USA, Jun. 25–30 (2012).

2. R. Kar, K. Hirao, "Do Long-Range Corrected Density Functionals Satisfy Koopmans' Theorem?", The 14th International Congress of Quantum Chemistry, Boulder, USA, Jun. 25–30 (2012).

3. A. Chutia, T. Tsuneda, "An examination of exchange-correlation functionals in solid-state calculations", 6th Annual Conference of the Molecular Science Society of Japan, University of Tokyo, Tokyo, Japan, Sep. 18–21 (2012).

4. R. K. Singh, T. Tsuneda, K. Miyake, M. Watanabe, " Theoretical Investigation of Proton Conductivity in Proton Exchange Membranes for Fuel Cells", 6th Annual Conference of the Molecular Science Society of Japan, University of Tokyo, Tokyo, Japan, Sep. 18–21 (2012).

5. J.-W. Song, K. Hirao, "An efficient hybrid DFT functional using a Gaussian attenuating HF exchange for band gap calculations of solid state materials", The 3rd AICS International symposium, Kobe, Japan, Feb. 28– Mar. 1 (2013).

(5) Patents and Deliverables

-None

18. Computational Disaster Mitigation and Reduction Research Unit

18.1. Team members

Muneo Hori (Unit Leader)

Hideyuki O-tani (Postdoctoral Researcher)

Jian Chen (Postdoctoral Researcher)

18.2. Research Activities

Computational disaster mitigation and reduction research unit is aimed at advancing large-scale numerical simulation for natural disasters such as an earthquake, tsunami and heavy rain, targeting 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 was launched at October 2012, and addressed the following research objects in this fiscal year:

1. Development of next-generation urban model for Kobe City

   An urban model is used as input data of natural disaster simulation. The reliability of simulations depends largely on its quality. We seek to develop a next-generation urban model for Kobe City; the current model is constructed, based on open-source data of a target area. More detailed data about the urban area, which area managed and maintained by local governments, will be used for the model.

2. Execution of large scale natural disaster simulation and smart visualization

   Utilizing the codes for Integrated Earthquake Simulation (IES) developed in SPIRE Field 3, we make a trial simulation for natural disaster simulation in Kobe City, for a given set of disaster scenarios. Urban area simulations based on the various scenarios generate massive information about possible hazards and disasters. One of the main researches of our unit is to consider smart visualizations of IES outputs so that Local Government can make use of the results of Science.

3. Development of advanced numerical methods for liquefaction and related problems

   Liquefaction is disastrous ground failure induced by earthquake. It refers to the change in ground behavior from solid to fluid. In the past, liquefactions due to strong ground motion have caused severe damages. Reliable predictions of liquefaction is thus of great significance, especially for regions important for human activities.

18.3. Research Results and Achievements

18.3.1 Development of next generation urban area model for Kobe City

In this fiscal year, we have developed an urban model of Kobe City as shown in Figure 1, utilizing the conventional schemes incorporated in codes for Integrated Earthquake Simulation (IES).

In IES, more than 100 thousands of building models are constructed automatically from GIS data, and the highest robustness is required in a methodology of converting GIS data to the building models. We are carrying out a preliminary study of a new methodology for the data conversion which is based on a template fitting operation. Figure 2 shows building models constructed by the

Figure 1: Next-generation urban model of Kobe city
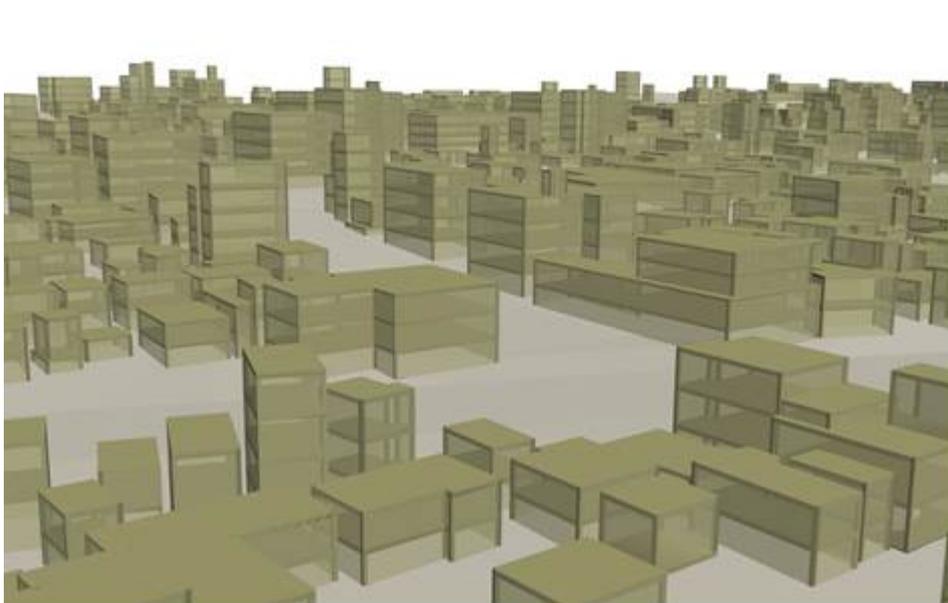
Figure 2: Building models for seismic analysis automatically converted from GIS data.

new methodology; more detailed models are generated, compared with the existing method.

18.3.2 Execution of large scale natural disaster simulation and smart visualization

We made a trial simulation for earthquake and tsunami, using the next-generation urban area model of Kobe City. In the earthquake simulation, more than 100 scenarios are considered. Since
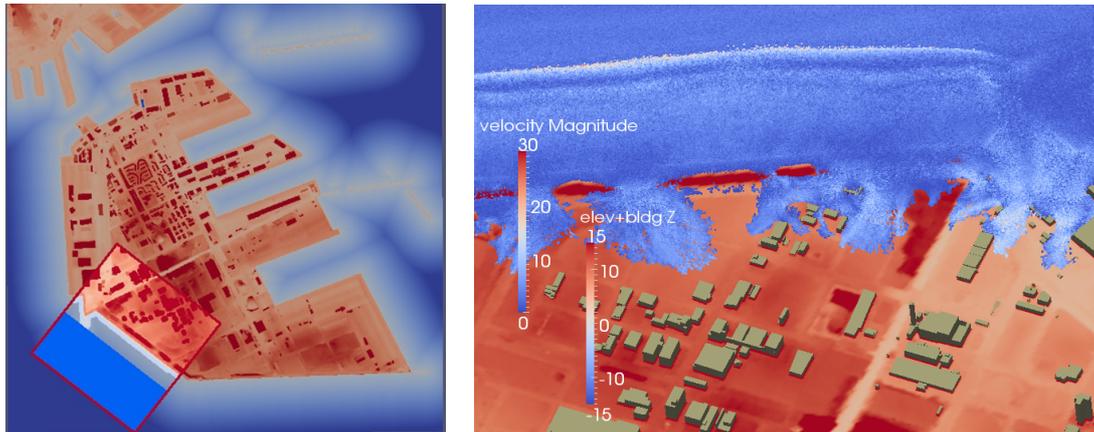
Figure 3: Trial simulation of tsunami attacking Port Island.　Left) model of Port Island; elevation data and building data are used, and the model is automatically constructed by using a data conversion module.　Right) snapshot of tsunami inundation on Port Island, when an extremely large tsunami height is assumed.
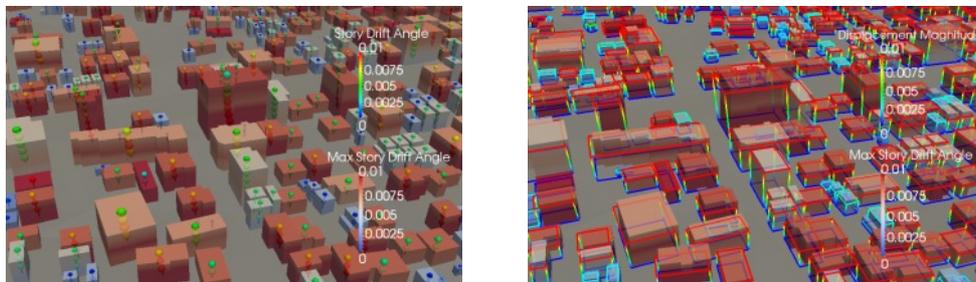
Figure 4: Dual visualizations for animation.
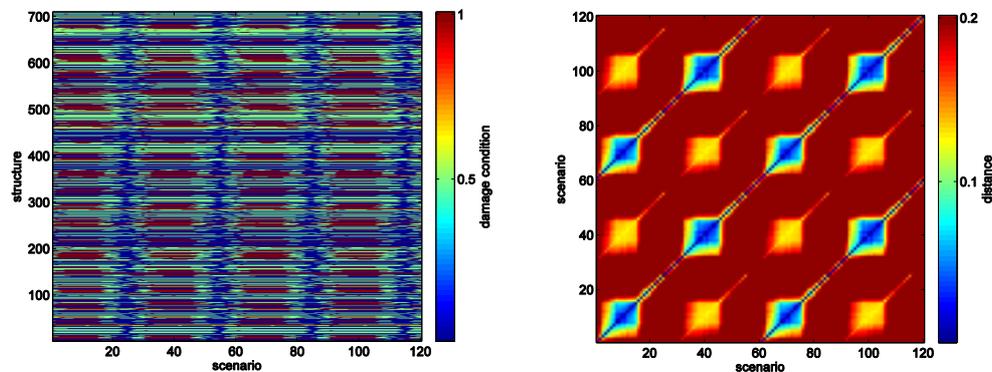
Figure 5: Pixel matrices for direct visualization of many earthquake scenarios. Left) damage conditions of all computed scenarios.　Right) a trial clustering of many earthquake scenarios.

simulation for one scenario generates results of 10TB, smart visualization methods are being studied. An input of the urban area hazard and disaster simulation is an output of hazard simulation that is made in the Japanese Island scale.

18.3.3 Development of advanced numerical methods for liquefaction and related problems

Key mechanism of liquefaction is non-linear coupling between soil and underground water, and it could be regarded as an instable phenomenon in the sense that shaking induces sudden transition from solid to liquid. A most advanced numerical method is required to analyze this phenomenon, which is able to chase the unstable solution.

18.3.3.1 Mathematical model

As the first step, we consider idealized mathematical model to analyze the stability of soil deformation and water pressure coupling problem. Denoting by $\boldsymbol{u}$ and p the perturbation of the soil displacement and water pressure, a mathematical model which describes liquefaction is expressed as

$$\begin{aligned} \rho \mathrm{D}^2\boldsymbol{u} - \nabla \cdot (\boldsymbol{c}{:}\nabla\boldsymbol{u}) + \nabla p &= \boldsymbol{0}, \\ \nabla \cdot \mathrm{D}\boldsymbol{u} - \nabla \cdot (k\nabla p) &= 0, \end{aligned} \tag{1}$$

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

Applying Fourier transform with kernel of $\exp{(\iota(\boldsymbol{\xi} \cdot \boldsymbol{x} - \omega t))}$, Eq. (1) becomes

$$\begin{aligned} -\rho\omega^2\boldsymbol{u} + (\boldsymbol{\xi} \cdot \boldsymbol{c} \cdot \boldsymbol{\xi}) \cdot \boldsymbol{u} + \iota\boldsymbol{\xi}p &= \boldsymbol{0}, \\ \omega\boldsymbol{\xi} \cdot \boldsymbol{u} - k(\boldsymbol{\xi} \cdot \boldsymbol{\xi})p &= 0. \end{aligned} \tag{2}$$

Here, for simplicity, the same symbols $\boldsymbol{u}$ and p are used for the transformed functions.

18.3.2.2 Theoretical and numerical analysis

For the isotropic case, it is readily shown that for any real-valued $\boldsymbol{\xi}$, ω becomes complex number but its imaginary part is always negative. This means that, due to coupling of soil deformation and water pressure, plane waves such as P- or S-wave decays. For the anisotropic case, however, the imaginary part of ω becomes positive for large anisotropy. Dilatancy, volume expansion due to shear stress, is a unique mechanical characteristic of soil, and can be regarded as anisotropy. Hence, this result suggests that as the degree of dilatancy increases, plane wave which accompany water pressure change could propagate in an unstable manner.

A numerical code which is able to analyze these two cases as well as the case of spherically propagating waves is being developed. The unique feature of this code is that it is able to model detachment of soil particles, which appears sharp drops in stiffness or elasticity.

18.4. Schedule and Future Plan

The unit has 5 years plan (2012-2016), and the first two years (2012-2013) are for the establishment of the unit. In this period, we seek to develop a prototype of a next-generation urban area model and its simulation methodology for multiple natural disaster scenarios, and to develop a prototype of an analysis method for liquefaction.

According to this schedule, in the fiscal year of 2013, we are going to construct a prototype of the next-generation urban area for Kobe City to carry out several natural disaster simulations using K computer. The results will be shared by local government as well as regional researchers. We are going to develop a prototype of liquefaction analysis, and examine the nature of instability of liquefaction by using large-scale numerical computation.

18.5. Publication, Presentation and Deliverables

(1)   Journal Papers

1.   Hideyuki O-TANI, Jian CHEN and Muneo HORI (2013): Smart Visualization of Urban Earthquake Simulation, *Journal of Japan Society of Civil Engineers, Ser. A1 (Structural Engineering & Earthquake Engineering (SE/EE))*, Vol. 69, No. 4.

(2)   Conference Papers
  -None

(3)   Invited Talks

1.   M. Hori, Application of large scale numerical computation to earthquake simulation, Seventh Gulf Seismic Forum 2012, Jeddah, Saudi Arabia 22-25 January

(4)   Posters and presentations

1.   Hideyuki O-TANI, Jian CHEN and Muneo HORI (2012): Smart Visualization of Urban Simulation, 32nd JSCE Earthquake Engineering Symposium.

2.   Hideyuki O-TANI, Jian CHEN and Muneo HORI (2012): Smart Visualization of Urban Simulation, The 3rd AICS International Symposium.

(5)   Patents and Deliverables
  -None

19.Computational Structural Biology Research Unit

19.1. Team members

Florence Tama (Unit Leader)

19.2. Research Activities

Biological molecular complexes of such as proteins and RNAs are of great interest in the area of molecular biology as they are involved in cell replication, gene transcription, protein synthesis, regulation of cellular transport and other core biological functions. Those systems undergo large conformational transitions to achieve functional processes. Therefore characterization of structures of these macromolecular complexes is crucial to understand their functional mechanisms, and play an important role in the development of new drugs to treat human disease.

Experimentally, X-ray crystallography has been the primary tool to study protein conformations, providing high-resolution structures. 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, it cannot achieve atomic level resolution such as obtained by X-ray crystallography. Indeed, theoretical work has shown that electron density maps of biological molecules could be obtained with resolution around 5 Å. Therefore; additional analyses on the XFEL data would be necessary to obtain atomic level structures.

Computationally, methods have been developed to predict structures from low-resolution data such as cryo-electron microscopy (EM) either using rigid body fitting or flexible deformations of known atomic structures. In addition, even when structures of the molecules are unknown, atomic models can be predicted using homology modeling and ab initio predictions. While, ab initio prediction still remains difficult for large proteins, success in predicting small proteins have been observed. Finally, algorithms to analyze protein/proteins interactions also have shown success in predicting proteins complexes.

Our research focuses on the development of computational tools to study biological systems, more specifically to help in their 3D structural determination using various experimental techniques and to analyze their potential interactions with small molecules in order to design new drugs.

The ultimate line of our interdisciplinary research is too bring experimental data as obtained from X-ray and XFEL with development and applications of computational tools through the K computer to acquire knowledge on the structure of a physiologically important protein complexes that are unattainable with existing experimental techniques, and to contribute to development of drug design

and medical treatment in collaboration with pharmaceutical companies.

19.3. Research Results and Achievements

The computational structural biology unit was established full-time in January 2013. The results presented here reflect the period from January to March 2013.

1. Cryo-EM qualitative fitting

Cryo-EM experiments produces low-to-medium resolution structures (usually in the range between 20 and 4 Å) but allows studying large (diameter larger than 10 nm and molecular weight sometimes of several mega-Daltons) and flexible macromolecular complexes inaccessible to X-ray and NMR techniques. Because the data is low-resolution, in order to obtain higher-resolution information, know X-Ray structure are often combined with cryo-EM data which is some cases requires X-ray structure deformation (flexible fitting). Flexible fitting of X-ray structure into cryo-EM maps requires first a rigid body fitting of the X-ray structure followed by deformation to fit the density map.

We have designed a new protocol for automating this process in order to obtain qualitative data on the accuracy of the fitting. Several starting rigid body fitting orientations are considered. In order to automatically identify a best orientation among the candidates obtained by rigid-body fitting, we performed flexible fittings using four different approaches starting with each of the candidate orientation. Models obtained from each fitting were then compared using a Root Mean Square Deviation (RMSD) as a measure. It is found that different flexibly fitting models only show consensus, i.e. low RMSD values, in conformation when the fitting procedures are started with a viable orientation (Figure 1).

This approach for identifying best orientation is an important step towards making the flexible fitting procedure fully automated. It is important to point out that the flexible fitting approaches used are themselves fully automated – they do not require any domain segmentations or human interactions. However, they require a suitable guess of the starting orientation, which requires human interactions or additional knowledge of the system. Our results shows that this requirement can now be eliminated and the whole fitting procedure can be automatized. As a result, the fitting procedure would only require initial structure and the target map. We are currently writing a paper describing those results.
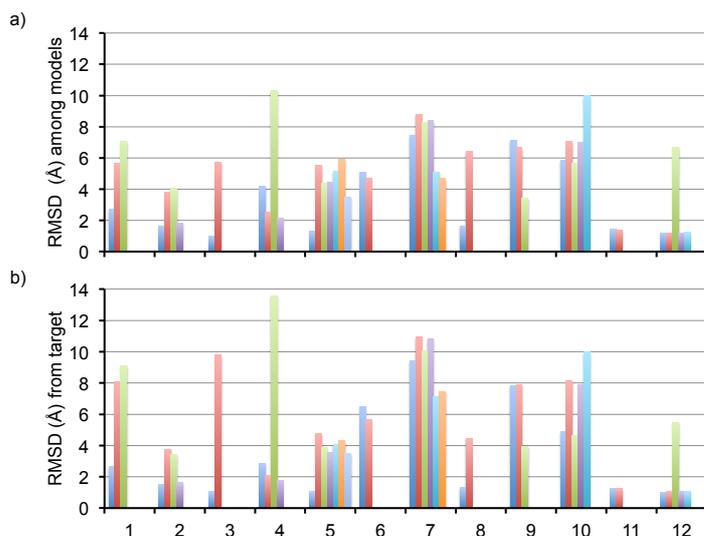
Figure 1: Mean of the pairwise RMSD among the four flexibly fitted models (panel a) and mean RMSD between the target structure and the four flexibly fitted models (panel b) using the different rigid body fitted orientations (representatives in colors) of the initial structure for each of the 12 proteins.

2. XFEL

During this fiscal year, the unit has also started discussions with researchers involved with XFEL experiments. Our unit has attended a workshop held a Keio University on XFEL. In addition, our unit visited the Harima site to observe XFEL experiments and discussed possible collaborations. These initial discussions have enabled us to identify several areas where our experience with cryo-EM data analysis could be pertinent with XFEL data analysis.

19.4. Schedule and Future Plan

We are planning on developing tools to analyze XFEL data, with special emphasis on the dynamics that can be extracted from the data. During the next fiscal year, we plan to make flexible fitting programs available to the community. XFEL data should provide low-resolution to medium resolution structural data. For an atomic description of the biological molecules, algorithms will be needed to deform known X-ray/NMR structures to fit correctly with the data from XFEL. The methods we have been developing for cryo-EM data will lay the foundation for this work. Such methods would allow investigating the role of the structural changes responsible for a protein function. Algorithms will be implemented within the Genesis program suite being developed specifically for K computer by Dr. Sugita (AICS RIKEN).

In addition, we plan to study extend of dynamics within raw low-resolution data. This research is an on-going collaboration with Dr. Slavica Jonic (CNRS, Paris). Macromolecular structure determination by cryo-electron microscopy (EM) and single particle analysis are based on the assumption that imaged molecules have identical structure. With the increased size of processed datasets it becomes apparent that many complexes coexist in a mixture of conformational states or contain flexible regions. Algorithms have been developed to yield estimates of voxel-by-voxel

variance of a structure reconstructed from the set of its projections. Such variances will be compared from enhanced sampling molecular dynamics simulations of biological molecules. Such type of approach could later on be extended to data from XFEL experiments as well.

On the longer term we plan to establish methodology to build structure from low-resolution structural data without a priori knowledge of the overall structure of the molecular complexes as potential targets of the structural analysis by XFEL are multiprotein/RNA complexes. Although it is difficult to acquire the crystal structure of the whole complex, the atomic structure of each component protein and RNA may be known. Moreover, for small proteins, even when there is no structure, their structures can be predicted in relatively high precision using homology modeling. Therefore, if such structures are correctly combined into a model of the complex that fits the three-dimensional electron density map obtained from XFEL, the atomic structure of a complex could be obtained. A computational framework using multiscale simulations, which would combine the representations at different resolution from all the atoms to coarse-grained representations as well as protein-protein docking algorithms will be developed for such purpose.

19.5. Publication, Presentation and Deliverables

(1)　Journal Papers

　　　-None

(2)　Conference Papers

　　　-None

(3)　Invited Talks

Understanding functions of biological molecules using hybrid methods, Feb 15th 2013 Department of Physics, Nagoya University

(4)　Posters and presentations

Characterization of large biological complexes using computational approaches and low-resolution experimental data. AICS 3rd International Symposium

(5)　Patents and Deliverables

　　　-None

20. System Operations and Development Team

20.1. Team members

Fumiyoshi Shoji (Team Head)

Atsuya Uno (Research & Development Scientist)

Hitoshi Murai (Research & Development Scientist)

Motoyoshi Kurokawa (Research & Development Scientist)

Keiji Yamamoto (Postdoctoral researcher)

Toshiyuki Tsukamoto (Research & Development Scientist)

Mitsuo Iwamoto (Technical Staff)

Katsufumi Sugeta (Technical Staff)

20.2. Research Activities

The K computer is a distributed-memory parallel computer system consisting of 82,944 compute nodes and has played a central role of the High Performance Computing Infrastructure (HPCI) initiative granted by the Ministry of Education, Culture, Sports, Science and Technology (MEXT). HPCI has achieved an integrated operation of the K computer and other supercomputer centers in Japan and has enabled seamless accesses of a cluster of supercomptuers including the K computer from users'machines. HPCI has also provided large-scale storage systems which can be accessed from all over Japan.

AICS provided computing resources to some advanced users as an early access to a part of the K computer from the end of March 2011 to September, 2012. During this early access,   the advanced users in five research fields of the Strategic Programs for Innovative Research (SPIRE) promoted by the MEXT implemented their application software. AICS could improve the system through their feedback. The K computer was completed in June 2012 and has been available for shared use since Septempber 28, 2012.

System Operations and Development Team (SODT) has conducted the research and development on advanced management and operations of the K computer. While analyzing the operational statistics collected duiring the shared use, SODT has improved the system configuration, such as the job scheduling, the configuration of the file system and users' environments. For example, it is very difficult to achieve higher system utilization because the K computer has to process various sizes and types of jobs simultaneously. SODT has responded flexibly to the user's requests and made analysis of the operational status, and then has realized high level utilization around 80%.

SODT also helps users handle the K computer and utilize the K computer resources effectively by improving the compilers, MPI libraries and other system tools. This support has been conducted together with the Software Development Team.

20.3. Research Results and Achievements

20.3.1. Improvements of system software of the K computer

We have fixed and improved many points of the system software since the beginning of the shared use. Here, we describe the main improving points.

➢ Job Scheduling

The K computer has to manage various types of jobs simultaneously, so it is very difficult to achieve a high level efficiency of compute node usage. We have analyzed the operational statistics collected during the shared use. Investigating the analysis result, we have improved the system software (such as the job scheduler, the file staging system, and so on) and decided to change the job scheduling policy as follows:

1. To assign the designated compute nodes to a small resource group for small size jobs using less than 384 compute nodes for preventing the small size jobs from disturbing the large scale job execution.

2. To make an exclusive period for the large scale job execution using more than 36,864 compute nodes to execute the large scale jobs smoothly.

As a result, we could improve the system usage and reduce the waiting time for the job execution (Figure 1).
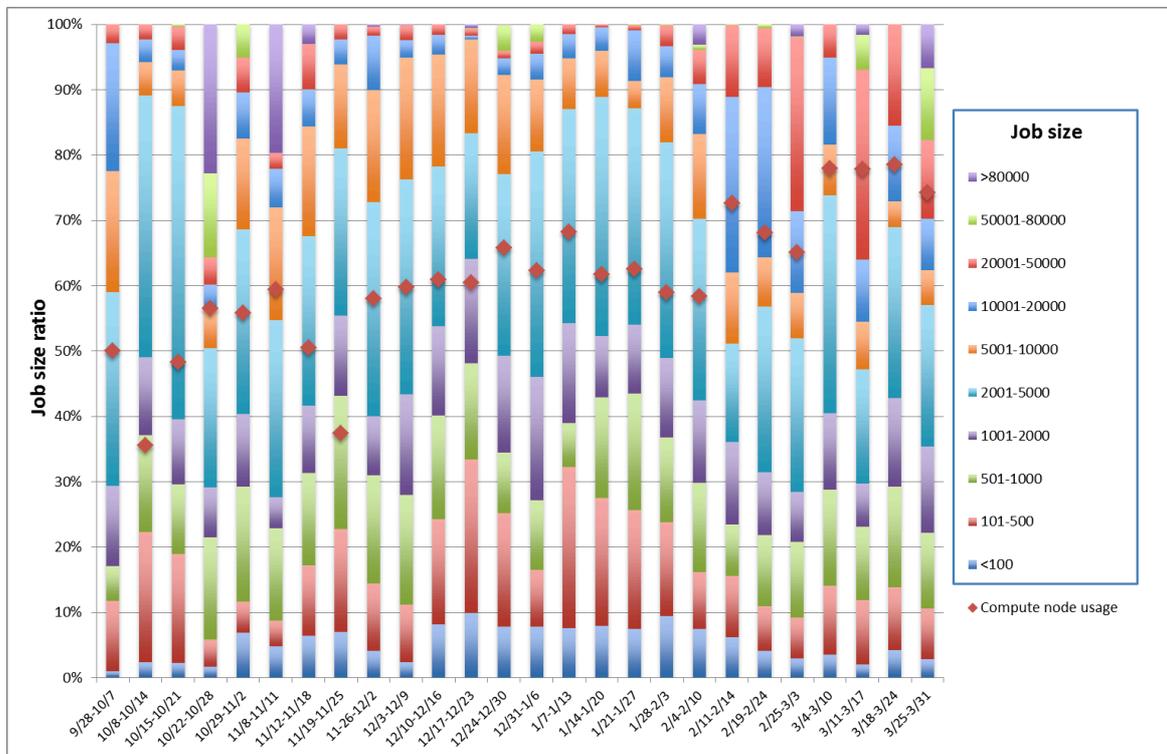

Figure 1 Details of resource usage during the shared use

Figure.1 indicates that the compute node usage has been improved and the number of executed large scale jobs has increased after changing the job scheduling policy on February, 2013.

➢ File system

The file system of the K computer is Fujitsu Exabyte File System (FEFS) based on Lustre file system and enhanced and tuned for the K computer. At the beginning of the shared use, we made 4 large volumes for user's home and data area. In this case, we required one month or more to check and repair the file system when an obstacle had occurred. This means that it is impossible to recover from the obstacles. So, we analyzed the users' usage and the setting of FEFS, and we decided to divide the file system to more smaller volumes and optimized the setting of FEFS. These changes enable to check and repair the files system within 48 hours without restrictions to users.

➢ Compilers, MPI libraries and System tools

Compilers and MPI libraries are customized and tuned for the K computer. But, through the shared use, we found the many improving points for them and improved them. These improvements have enabled the user to improve the performance of the user's application without any code changes. In figure 2, the performance of original Alltoallv and improved Alltoallv on the K computer are shown. This graph indicates that the improved Alltoallv is about 4 times as fast as original one using 10KB message size.
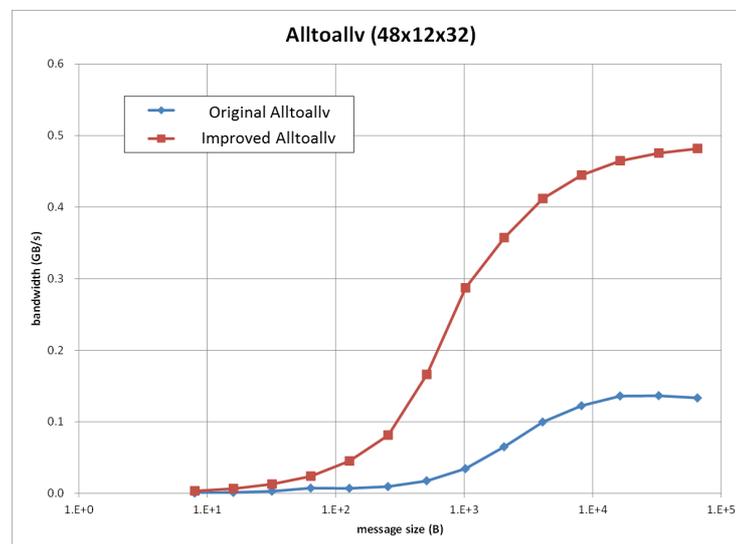

Figure 2 Performance of Alltoallv on the K computer

Many users request for tools that support the use of the K computer, so we are developing the tools as follows:

1. To provide the estimated waiting time for the job execution

155

2. To provide the available node information of the job execution
3. To provide the confusion information of the compute nodes

We consider these tools will be useful for the users.

20.3.2. User support

We have conducted the user support, such as the user management and the consulting services.

➢ User management

The K computer has 120 or more groups and 1,400 or more users at the end of March, 2013. The most of users are HPCI users and the members of AICS research divisions also study using the K computer. HPCI system performs the user management of HPCI users aside from us, so we have to adjust the difference between HPCI system and the K computer. We have developed the user managing system for this, and it enables to perform the user management of HPCI users and AICS users in the same way.

➢ Consulting services

We support users through "the K support desk" and provide users the technical information on the K computer including system environments, system tools, and software libraries. The consulting services have been conducted together with the Software Development Team. The consultation number in the period from the beginning of the shared use to the end of March, 2013 is approximately 1,400.

20.4. Schedule and Future Plan

We continue to improve the system software of the K computer and to provide the user support, and we will release the system tools that support the use of the K computer in FY2013.

20.5. Publication, Presentation and Deliverables

(1) Journal Papers

   - None

(2) Conference Papers

1. Daisuke Takahashi, Atsuya Uno and Mitsuo Yokokawa: An Implementation of Parallel 1-D FFT on the K computer, HPCC2012, 25-27 Jun. 2012, Liverpool, UK.
2. T. Boku, K.-I. Ishikawa, Y. Kuramashi, K. Minami, Y. Nakamura, F. Shoji, D. Takahashi, M. Terai, A. Ukawa, T. Yoshie: Multi-block/multi-core SSOR preconditioner for the QCD quark solver for K computer, The 30th International Symposium on Lattice Field Theory, June 24-29, 2012, Cairns, Australia.

(3)   Invited Talks

1.   M.Kurokawa: The K computer and Expectations for Optical Devices, The Joint International Symposium on Optical Memory and Optical Data Storage 2012, 30 Sep.- 4 Oct. 2012.

2.   M.Kurokawa: The K computer: 10 Peta-FLOPS supercomputer, 10th International Conference on Optical Internet (COIN), 29-31 May 2012.

3.   F.Shoji: The K computer -System and Applications-, The 41st International Conference on Parallel Processing, Sep 10-13 2012, Pittsburgh, PA, USA.

(4)   Posters and presentations

1.   Atsuya Uno, Fumiyoshi Shoji and Mitsuo Yokokawa: The performance evaluation of the job scheduling with the file staging, IPSJ-SIGHPC 2012-HPC-136(22), 2012. (In Japanese)

(5)   Patents and Deliverables

    - None

21. Software Development Team

21.1. Team members

Kazuo MINAMI (Team Head)

Masaaki TERAI (Research & Development Scientist)

Atsuya UNO (Research & Development Scientist)

Akiyoshi KURODA (Research & Development Scientist)

Hitoshi MURAI (Research & Development Scientist)

Kiyoshi KUMAHATA (Research & Development Scientist)

Shunsuke INOUE (Research & Development Scientist)

Yukihiro HASEGAWA(Research & Development Scientist)

Shinji HAMADA (Postdoctoral Researcher)

21.2.Research Activities

Applications that use calculative resources to the maximum and high system performance are essential elements of the K computer that can run applications for parallelization on a scale of several tens of thousands. Our team selected, from the development stages of the K computer, six target applications that are expected to contribute to the advancement in the numerical simulation and computer engineering fields, and we promoted research and development for increasing their performance.

Further, in order to make applications perform at a high level, it is also necessary to increase the functionality and performance of the system as well as middleware. By evaluating and improving these areas, we are further promoting enhancements in the operation of the K computer. During 2012, the following actions took place in line with the above principles.

(1) Performance testing of the K computer systems as a whole using real applications

Towards completion of K computer in June 2012, we performed 10PFLOPS system performance testing using the aforementioned six target applications.

(2) Systematization of methods for increasing application performance in the K computer

Methods of increasing performance differ according to the features of the application, such as memory access patterns, required BF values, and parallel characteristics. We organized these in terms of each feature and systematized methods for improving performance.

(3) Support for consultations on usage by the registered institution

We fielded questions regarding application performance from the registered institution/AICS research departments. Further, we provided support for the necessary methods to increase performance, in order to draw out the CPU performance and parallel performance of the K

computer.

(4) Increased sophistication of compiler tools of the K computer and procedures of methods to increase performance

We increased the efficiency of compiler tools in order to make (1), (2), and (3) more efficient. In addition, we established methods such as kernel segmentation, performance prediction methods during times of high levels of parallelization and debug methods, and created procedures and tools for these.

21.3.Research Results and Achievements

21.3.1 Performance testing of the K computer system as a whole using real applications

In order to carry out performance testing on the K computer system as a whole, we selected six applications from each application field, with different computational and scientific characteristics. (Fig 1)

Program Name	Discipline	Application Overview	Expected Results	Scheme
NICAM	Earth Science	Nonhydrostatic icosahedral atmospheric model	Dramatically advance simulation by subtly expressing tropical cumulus convection activities that serve as the engine to atmospheric general circulation, making it possible to clearly explain atmospheric phenomena that are difficult to reproduce today.	FDM (atmosphere)
Seism3D	Earth Science	Seismic wave propagation / strong seismic motion simulation	Make it possible to analyze and predict the motion of seismic waves of a short period not feasible with existing computers, making application to the evaluation of earthquake resistance of wooden buildings and concrete structures possible.	FDM (wave)
PHASE	Material Science	Plane wave expansion first-principle molecular dynamics analysis	Explore post 35-nm generation nano-devices and non-silicon devices via first-principle calculations.	DFT (plane wave)
FrontFlow/blue	Engineering	Unsteady flow analysis based on large eddy simulation (LES)	Make it possible to make high-precision flow predictions, including behavior predictions of the turbulent boundary layer critical to engineering.	FEM (fluid)
RSDFT	Material Science	Real-space first-principle molecular dynamics calculation	Analyze the characteristics of basic nano elements (quantum wires, molecules, electrodes, gates, infrastructures, etc.) of 10-nm or less using large-scale first-principle calculations.	The Real-space DFT
LatticeQCD	Physics	Lattice QCD simulation based elementary particle and nucleus research	Clearly identify the origins of matter and the universe using the Monte Carlo method and CG method.	QCD

Figure 1 Six applications

By focusing on the unified use of the 10PLOPS scale, we used these applications to evaluate the 5 items of calculative performance, inter-node communication performance, I/O performance, staging performance, and performance hindering factors.

A) Calculative performance

We evaluated node unit performance, which determines K computer computational performance. From the weak scale measurement results, which are equivalent to the computational volume per node, we confirmed that there was no performance degradation when executing 10PFLOPS. The application uses NICAM, QCD. With NICAM, an increase in execution time and performance degradation was observed when processing 81,920 parallel processes. A survey revealed that the read processing of data within the evaluation area was the cause, and we confirmed that performance degradation could be avoided by excluding this.

B) Inter-node communication performance

We evaluated communication performance between nodes, which strongly affects the parallel performance of processes. We compared the fundamental performance (ideal measurement value obtained through benchmarks) of the MPI communication measurement value obtained through running the applications, and confirmed that the communication performance between nodes can be achieved, as designed, on a 10PLOPS scale. The application uses RSDFT, Seism3D and FFB. With RSDFT, the Tofu-dedicated algorithm Trinaryx3 is operated for collective communication Allreduce, Bcast and Reduce, and we confirmed that the bandwidth specified for fundamental performance was achieved. With Seism3D and FFB, we confirmed that the adjacent communication isend/irecv measurement values specified for fundamental performance were achieved.

C) I/O performance

We evaluated the I/O performance with the local file system during execution of the application. We confirmed the actual values measured when executing the application with the fundamental performance, and confirmed that I/O performance can be obtained. The application uses NICAM. In terms of file input, the actually measured throughput value was high, but it was estimated that this was actually carried out on only a section of the data and judged to be adequate. In terms of file output, as the throughput value is the same as fundamental performance, performance is considered to be adequate.

D) Staging performance

After execution of the application, we evaluated file transfer between the global file system and the local file system. When executing the application, we compared the actual measured value from staging with fundamental performance, and confirmed that it achieved the same level of performance. The application used RSDFT, PHASE and NICAM. It was inefficient in the case of RSDFT, PHASE, where transfer size is small, and performance was low. However, with NICAM, where the transfer size was larger at 32 GB, adequate performance was obtained, being at the same level as fundamental performance.

E) Performance hindering factors

We confirmed whether there was any performance degradation caused by OS jitter or any external

factors. Using FFB, Seism3D, QCD and RSDF, we confirmed load balancing between the processes and also confirmed that there were no issues.

21.3.2.Systematization of methods of increasing application performance with the K computer

The six applications used in 3.1 are defined on the basis of the following computational science characteristics.

- In regard to high parallelization, can strong parallel performance be achieved with a comparatively simple parallelization method? Alternatively, is it impossible to achieve high parallelization without using a complex parallelization method?

- In regard to improving the performance levels of unit performance, does achieving high unit performance with current computers tend to be difficult because of the high ratio of memory band width and floating-point arithmetical operations required by the application? Alternatively, does achieving comparatively high levels of unit performance tend to be easy because of low B/F values being required by the application?
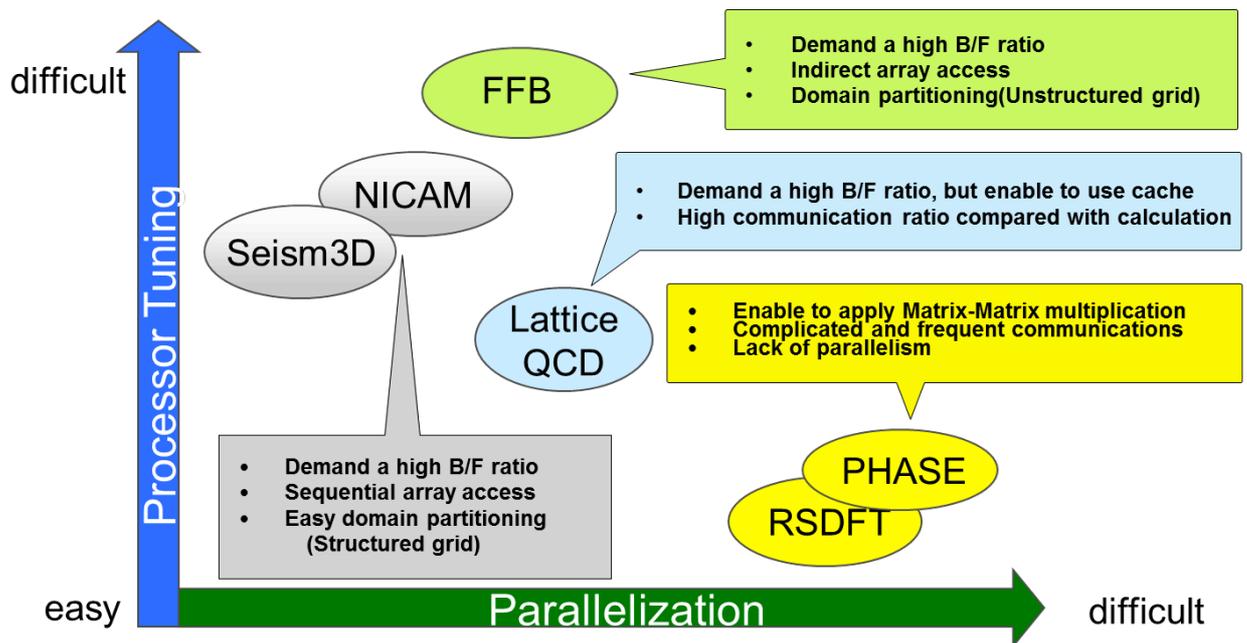

Figure 2 Behavior in Computational Science

In Fig 2, each application is plotted on the two evaluation axis. The methods for improving the performance of the applications were systematized as described below based on these computational science features.

161

A) NICAM, Seism3D group

In regard to high parallelization, a simple parallelization method based on adjacent communication is used, thereby making it easy to achieve strong levels of parallel performance. The K computer network topology is like a structured grid with 1 hop communication guaranteed for adjacent communications in 6 directions, and the design is such that the cost associated will not increase with high parallelization. No increase in communication cost was seen when validating the K computer's full nodes using Seism3D where adjacent communications occur in 4 horizontal directions.

Further, in regard to increasing the performance levels of unit performance, as the required B/F is high despite continuous access, it is difficult to achieve high levels of unit performance. With this type, it is first important to confirm that the practical memory bandwidth of the hardware in the hotspot loop is achieved. Causes of this not being achieved include L1 cache slashing or register spills due to stream variables and scalar variables being described in high volumes in the innermost loop. These can be effectively avoided using loop division and array merging.

B) PHASE, RSDFT group

With the original code, restrictions to the application mean that parallelization on the scale of several tens of thousands were not impossible for this group. RSDFT, in addition to traditional space division, has implemented division in the direction of the energy band. PHASE, in addition to traditional energy band division, has rewritten the application as one that can handle high parallelization execution to the tune of several tens of thousands through the addition of wave number direction division. Further, as these applications make heavy use of group communications and there is a high volume of traffic, the focus at times of high parallelization is how the K computer network topology or high speed library are used. With RSDFT, as there is a high volume of traffic each time, the group communication algorithm Trinaryx3 for Tofu is used. With PHASE, high speeds are achieved by packing all the traffic within a small scale of partial space through bi-axial parallelization, thus controlling the share of large-scale total traffic.

Further, from the viewpoint of increasing performance levels of unit performance, as, in principle, it is possible to rewrite the matrix–matrix product, the use of rewrite tuning in order to use matrix–matrix product libraries (DGEMM) is effective.

C) FFB group

As this type is based on list access and has a high request B/F, the important thing in terms of improving unit performance is to what extent the list data can be stored in the cache. With FFB, the analysis space is divided into small spaces, tuning was performed in which vector data is stored in the cache by renumbering within the small space. In regard to high parallelization, we need to focus on how Allreduce transitions as a result of an increase in the parallelization on the unstructured grid. However, when using the hardware barrier function of Tofu interconnect, a value close to fundamental performance was confirmed even on a full node scale.

D) LatticeQCD group

Despite traditionally having high B/F requirements, as it can operate on-cache, it is easier to achieve unit performance than with the FFB or Seism3D, NICAM group. However, with QCD, we observed an increase in L1 cache misses and integer load cache access waits, and sluggishness in the rise of the SIMD command rate. In regard to these issues, the expected performance could be achieved by improving the compiler or using the SIMD embedded function.

Through the use of these methods, the performance described in Fig3 has been achieved.

Program Name	PFLOPS/ Peak Ratio	Used Node							
			Calculation				Communication		
			Operation count	Byte/Flop	Memory access		Type	Frequency	Data Size
NICAM	0.24Pflops/ 9.23% [1]	81,920	$O(N)$ N:mesh	high	sequential access		neighbor hood	few	small
Seism3D	1.90Pflops/ 17.9%	82,944	$O(N)$ N:mesh	high	sequential access		neighbor hood	few	small
PHASE	2.14Pflops/ 20.2%	82,944	$O(N^3)$ N:atoms	low	sequential access		collective	many	large
FrontFlow/blue	0.31Pflops/ 3.16% [2]	80,000	$O(N)$ N:mesh	high	list access		collective	few	small
RSDFT	5.48Pflops/ 51.7%	82,944	$O(N3)$ N:atoms	low	sequential access		collective	many	large
LatticeQCD	1.57Pflops/ 15.6%	82,944	$O(L^5/a^7)$ L: lattice size a: grid space	high	sequential access		neighbor hood	many	small

[1] Result of 20,480 nodes. Result of 81,920 is confirming now.
[2] We are continuing performance tuning.

Figure 3 Feature of six application and achieved performance

21.3.3. Support for consultations on usage by registration institute

A) Hold an exchange of opinions in regard to increasing the sophistication of applications with registration agencies

Meetings for the exchange of opinions were held with the aim of sharing skills in relation to increased sophistication of applications with the registered institution. (10/2, 10/31) The content mainly involved the introduction of examples, such as methods of analyzing cost on the K computer, methods of judging tuning spots and tuning methods, and those in charge of increasing speed on both sides found the discussion beneficial.

B) Support for the use of K computer

In terms of user support, as a wide area of support is requested ranging from the K computer system to software technology, this will be provided in collaboration with the system operation and

development team. In the operational technology department, a user support service, named K support desk, is provided from the test usage period, and this will continue to be used after joint use begins.

The K support desk provides support for the technically specialized questions among the general usage issues transferred from the registration period, and framework issues related to the adjustment and increased sophistication of the K computer, mainly for the research departments of AICS. Further, as part of the operation, work is carried out periodically to check the status of responses to inquiries, in order to promote the smooth handling of questions and issues, and investigate necessary issues related to increased sophistication in the future. In the 6 month operating period from the start of shared use until the end of March 2013, it dealt with approximately 1400 inquiries.

21.3.4. Sophistication of compiler tools and procedures for methods to improve performance using the K computer

A) Advancements in the compiler runtime system

We discovered performance issues in the compiler and runtime system from the perspective of the aforementioned six applications and increasing speed, using the supported user applications. We further carried out improvement testing. These items will be reflected in the actual operating environment within this year.

1. As following condition, automatic parallelization is not performed when optimization control specifier "noreccurrence" is specified.
   - There is operation between for block and for block with nested loop.
   - Loop index variable is depends on the variable which is used in the out of loop body.
2. Removal of restriction that software pipelining is not work when XFILL optimization is applied.
3. Amendment that simd optimization is performed using "-Ksimd=2" option even when there is reduction operation in if clause.
4. Simd optimization is applied to ibits function.
5. Deterrence of relocate of dynamic linker for a purpose of control dispersion of execution time.

B) Increased sophistication of the profiler

We are providing a profiler (PA function) that uses the CPU event counter function to our K computer users and we have worked to increase the sophistication of this PA function. With the PA function up until 2011, the measurement location resource usage information (memory bandwidth, peak performance ratio, cache miss rate, SIMD rate etc.) was displayed as numerical data or ratios on a graph, but it was difficult to judge the area in which tuning should be applied for each user. In the advancements on this occasion, we have realized a level of visualization with greater PA

output legibility than now, by coloring the number cells on which the user should concentrate, adding indicators and clarifying bottleneck points etc., thus guiding you to the next tuning step.

C)   Procedures for methods of improving performance

In regard the work to generally improve the speed of applications, it took a lot of effort to grasp the logical structure. As a plan to resolve this, we have developed a static analysis tool (K-scope) with the aim of providing code reading support for the purposes of tuning.

The K-scope is constructed in Java and will operate in an ordinary PC environment. It has the adopted the interface shown in Fig4. This provides the analysis results with the program logical structure is shown in a tree structure on the left-hand side, the source code for the selected area shown on the top right and the list of variable features and floating point counts etc. shown on the bottom right. The plan is to publish this software as open source in April 2013.
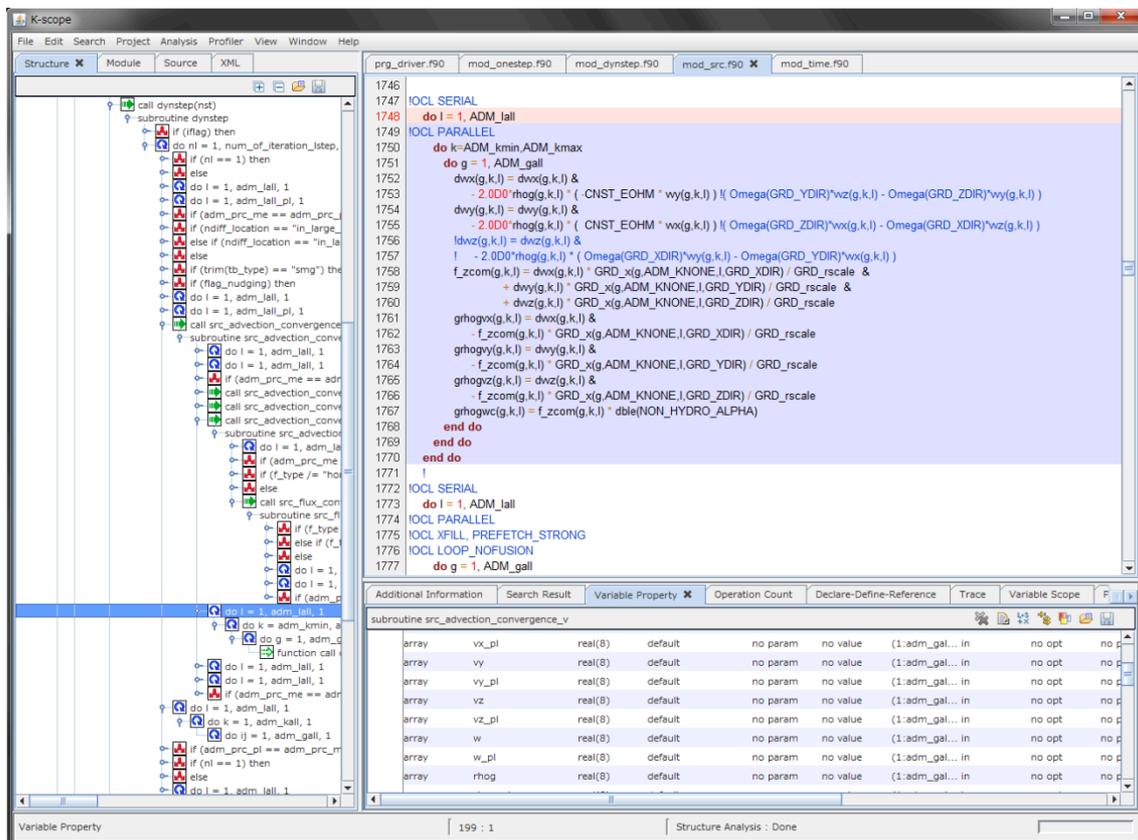

Figure 4 Snapshot of K-scope

21.4. Schedule and Future Plan

We will continue to further analyze and evaluate the K computer hardware, compiler features and computational science features of the applications, and systematize methods of increasing their

sophistication. Further, aiming to provide an environment in which it is easy for users to use the K computer, we will continue to promote advancements in the middleware used by the application.

21.5. Publication, Presentation and Deliverables

(1) Journal Papers

  - None

(2) Conference Papers

1. M. Terai, E. Tomiyama, H. Murai, K. Minami and M. Yokokawa, "K-scope: a Java-based Fortran Source Code Analyzer with Graphical User Interface for Performance Improvement", 41st International Conference on Parallel Processing Workshops, September, 2012.

2. M. Terai, K. Ishikawa, Y. Sugisaki, K. Minami, F. Shoji, Y. Nakamura, Y. Kuramashi and M. Yokokawa, "Performance Tuning of a Lattice QCD code on a node of the K computer", High Performance Computing Symposium 2013,January (2013). (in Japanese)

3. S. Inoue, S. Tsutsumi, T. Maeda and K. Minami, "Performance optimization of seismic wave simulation code on the K computer", High Performance Computing Symposium 2013, January, 2013. (in Japanese)

4. K. Kumahata, S.Inoue and K. Minami, "Performance Tuning for Gradient Kernel of the FrontFlow/blue on the K computer", High Performance Computing Symposium 2013, January, 2013. (in Japanese)

5. A. Kuroda, Y. Sugisaki, S.Chiba, K.Kumahata, M. Terai, S. Inoue and K. Minami, "Performance Impact of TLB on the K computer Applications", High Performance Computing Symposium 2013, January , 2013. (in Japanese)

(3) Invited Talks

1. K. Minami, "Massively Parallelization and Performance Improvement of Applications on the K computer", Symposium on Advanced Computing Systems and Infrastructures 2012, May, 2012. (in Japanese)

2. K. Minami, "Overview of Development of the K computer and Prospects for the Future", Kure Medical Association lecture, November , 2012.(in Japanese)

3. A. Kuroda, K. Minami, T. Yamazaki, J. Nara, J. Kouga, T, Uda and T. Ono "Can we speed up of FFT on Massively-parallel architecture? ", The 3rd society for Computational Materials Science Initiative , December, 2012. (in Japanese)

4. Y. Hasegawa, "Toward Petaflops Applications - First-principles electronic structure calculation program RSDFT -",   HPC Strategic Program Field 5   "The origin of matter and the universe" Symposium, March, 2013.(in Japanese)

5. A. Kuroda, "Example of Utilization of the K computer - With Optimization of PHASE", The Society of Polymer Science, Research Group on Computational Polymer Science, March,2013.(in Japanese)

(4) Posters and presentations

1. K. Minami, "Parallelization and Performance Improvement of Applications on the K computer", RIKEN Seminar, July, 2012. (in Japanese)

2. A. Kuroda, "Can we speed up of FFT on the K computer? -- With Performance Optimization of PHASE--", RIKEN Seminar, July, 2012.(in Japanese)

3. Y. Hasegawa, "Development of Petaflops Application RSDFT", RIKEN Seminar, July, 2012.(in Japanese)

4. K. Minami, "Optimization Ⅱ", AICS Summer School, August,2012. (in Japanese)

5. K. Minami, "Performance of Real Applications on the K computer", Computational Science Seminar, August, 2012. (in Japanese)

6. A. Kuroda, K. Minami, T. Yamasaki, J. Nara, J. Koga, T. Uda, and T. Ohno, "Planewave-based first-principles MD calculation on 80,000-node K-computer", SC'12, November, 2012.

7. K. Minami, "Performance Improvement of Applications on the K computer", SC'12, RIKEN AICS Booth Short Lectures, November, 2012.

8. Y. Hasegawa, "Effective use of collective communications tuned for the K computer in the real-space density functional theory code", SC'12, RIKEN AICS Booth Short Lectures, November, 2012.

9. M. Terai, E. Tomiyama, H. Murai, K. Kumahata, S. Hamada, S. Inoue, A. Kuroda, Y. Hasegawa, K. Minami and M. Yokokawa, "Development of supporting tool "K-scope" to tune of Fortran code", High Performance Computing Symposium 2013, January, 2013. (in Japanese)

(5) Patents and Deliverables
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