RIKEN AICS
Annual Report FY2016
AICS Research Activities

March 7, 2018

Preface

Welcome to the RIKEN AICS Annual Report for 2016. Five years have passed since the official operation of the K computer. In many areas we see many great results. We are very excited about this annual report that illustrates the significant accomplishments that our AICS teams have achieved this year.

The K computer has been demonstrated an extraordinary level of stability and provided exceptional service to science, engineering, and research communities. This is due to the dedicated efforts of the teams of the operations and computer technologies division.

RIKEN AICS, is the Japanese flagship research institution in computational science, founded in 2010 and is meant to be the COE for various simulation fields such as biology, physics, chemistry, weather and climate, disaster mitigation, cosmology, engineering, etc. We also focus on computer science research such as processor design and system software as well as fundamental technologies including programming framework and visualization. We would like to lead the world in achieving new research and development through scientific excellence.

The K computer significantly enhanced the resolution both in precision and spatial and temporal sizes through massively parallel computation. In addition, capacity computing opened the possibility of prediction in complex phenomena and optimization in multi-dimensional spaces. The K computer significantly enhanced the capacity computing in addition to the capability computing.

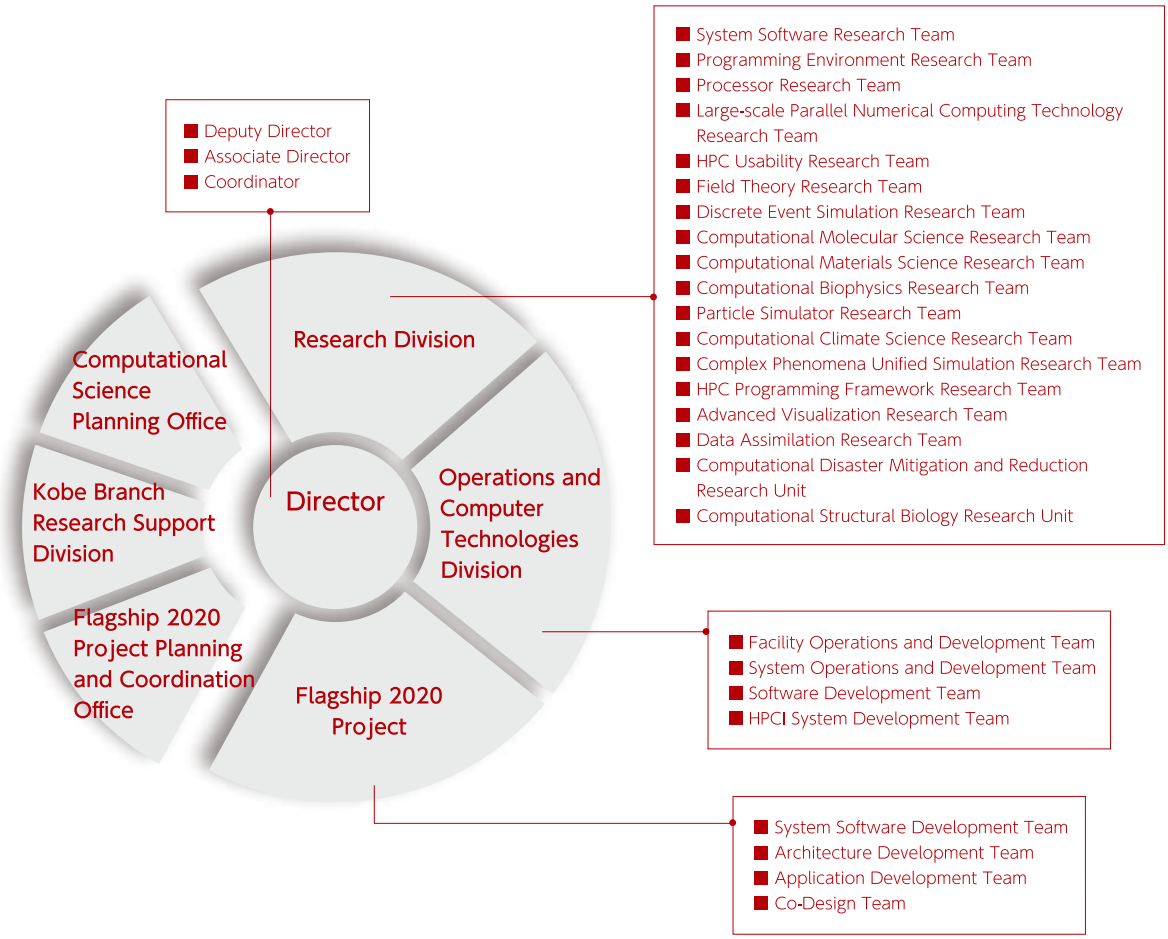
Continued development of world top-class supercomputer is vital for the world leadership in science and technology. AICS is now developing a world's top-class supercomputer, "post K", launching in around 2020 to spearhead the quest for knowledge of human kind.

Big data and big simulation are both essential elements of an integrated computing research and development. There are great opportunities and challenges in advanced computing, in both simulation and data analysis. Scientific discovery via computational science and data analytics is truly the "endless frontier".

We hope you enjoy reading all the wonderful advances made by RIKEN AICS. We look forward to continuing our activities for more fundamental and bigger science and engineering for years to come.

Kimihiko Hirao, Director

Organization



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Part I

Research Division

This report presents the research activity of the Research Division of RIKEN Advanced Institute for Computational Science (AICS) for the period of 1 April 2016 to 31 March 2017.

This is the seventh year for AICS since its foundation in 2010. The Research Division operated with 16 teams and 2 units. As of 1 April 2015, the number of researchers in the Division was 125 in total.

The research activity in this fiscal year resulted in 99 journal papers, 126 conference reports, 32 invited talks, 267 posters and presentations, 34 patents and deliverables.

Memorable awards bestowed upon AICS researchers included No. 1 ranking on Graph500 in June and November 2016, continuing the streak of top ranking since June 2015, and No. 1 ranking on HPCG garnered in November 2016 from the 2nd ranking in June. Top500 ranking became 5th in June and 7th in November 2016. Taken together, those rankings continued to illustrate the well-balanced and versatile performance of the K computer in its 5th year of operation.

Many research-related events took place in this fiscal year. The 7th AICS International Symposium, which became an annual event at Kobe, was held on 23-24 February 2017 under the title "Emerging numerical techniques for exascale and post-Moore era". 6th JLESC Workshop, a biannual series of workshops promoting research collaboration among 6 HPC institutions of Joint Laboratory on Extreme Computing, was held on 30 November-2 December 2016 for the first time in Kobe. RISDA2017, "RIKEN International Symposium on Data Assimilation", held on 27 February - March 2017, internationally promoted data assimilation research rapidly growing at AICS. RIKEN AICS HPC Youth Workshop held on 28-30 November was a new style of workshop for young researchers in which all participants made presentations and discussions in a group format mentored by senior but young AICS researchers.

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

December 2017

Akira Ukawa
Research Division Director
and Deputy Director
RIKEN Advanced Institute for Computational Science

Chapter 1

System Software Research Team

1.1 Members

Yutaka Ishikawa (Team Leader)

Atsushi Hori (Senior Scientist)

Yuichi Tsujita (Research Scientist)

Masayuki Hatanaka (Research Associate)

Toyohisa Kameyama (Technical Staff)

The system software research has been conducted in cooperation with the following members of the System Software Development Team in the Flagship 2020 project.

Yutaka Ishikawa (Team Leader)

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Atsushi Hori (Research Scientist)

Balazs Gerofi (Research Scientist)

Masayuki Hatanaka (Research & Development Scientist)

Takahiro Ogura (Research & Development Scientist)

Tatiana Martsinkevich (Postdoctoral Researcher)

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 toward exa-scale computing. We have been mainly focusing on scalable high performance communication and file I/O libraries and/or middlewares. The former research topics, sharing virtual address space and IHK/McKernel light-weight kernel, have been almost taken over by the System Software Development Team, but the research results are shown here.

1.3 Research Results and Achievements

1.3.1 PRDMA

The goal of this research is to design and evaluate an efficient MPI implementation for neighborhood communication by taking advantage of the Tofu interconnect, which has multiple RDMA (Remote Direct Memory Access) engines and network links per MPI process. The neighborhood communication pattern is commonly used in the

ghost (or halo) cell exchanges. The PRDMA (Persistent RDMA) is an enhancement of MPI persistent point-to-point communication primitives to reduce the communication latency and to improve the overlap between computation and communication over an RDMA-enabled interconnect. The MPI persistent point-to-point communication is defined in MPI standard since MPI version 1.1 specification. The RDMA-based transfers can progress the non-blocking communication without CPU intervention after synchronizing with the remote peers, and reduce extra copy overheads and memory consumption for data transfers due to the Zero-Copy feature. For example, when calling with the same communication parameters from an iterative stencil loop, the persistent communication can avoid the redundant setup cost on every call, including the RDMA buffer address exchanges. Also, the initial costs to optimize the communication can be amortized over a number of stencil iterations.

We implemented the prototype of the PRDMA protocol over the Open MPI provided on the K computer in FY2012. In FY2013, we improved the performance in the ghost cell exchange pattern, such as derived datatype handling and special handling upon non-periodic boundary condition. In FY2014, we applied the PRDMA to an optimized prototype implementation of MPI-3 neighborhood collectives, such as `MPI_Ineighbor_alltoallw`, over MPICH on the K computer. In FY2015, we improved the quality of the MPICH on K computer, and made it available for public use on the K computer. In addition, we have been implementing the prototype of the PRDMA-based MPI-RMA implementation on the Tofu2 interconnect of FX100 to compare with the MPI-3 neighborhood collectives.

In FY2016, we implemented the persistent neighborhood *alltoall* collective primitives, being standardized at the MPI Forum, on the FX100 Tofu2 interconnect[1]. The implementation uses the new offloading feature of Tofu2 to allow it to offload the entire PRDMA protocol on the hardware, including process synchronizations between sender and receiver. Thus, it allows truly asynchronous progress of communication without any progress threads.

```
01 while (iterations--) {
02   MPI_Barrier( );
03   t[0] = MPI_Wtime();
04   MPI_Start( &preq );
05   t[1] = MPI_Wtime();
06   /* no sleep */
07   t[2] = MPI_Wtime();
08   MPI_Wait( &preq );
09   t[3] = MPI_Wtime();
10 }
```

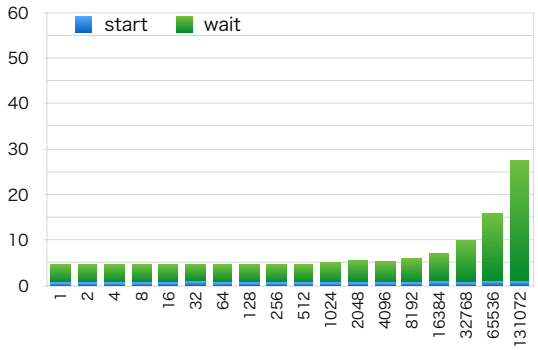
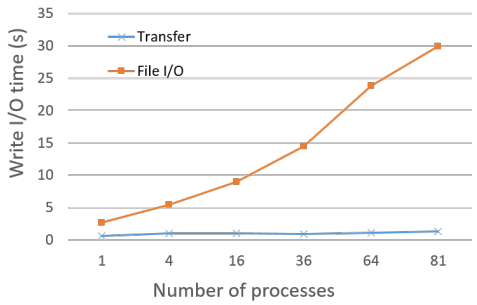


Figure 1.1: Benchmark Result of Persistent Neighborhood All-to-All

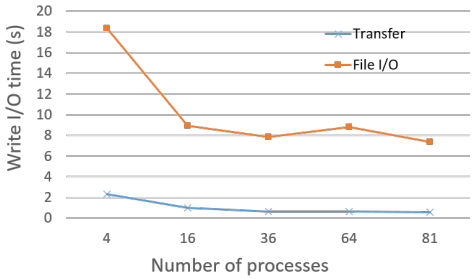
Figure 1.1 shows a benchmark result of the persistent neighborhood *alltoall* collective operation on FX100. The benchmark uses a latency benchmark program as illustrated in the left figure of Figure 1.1 and the communication pattern of ghost region updates in two dimensional five-point stencil computation. In the right figure, the horizontal axis indicates the message length in bytes, and vertical axis indicates the latency in microseconds. The graph in the right figure illustrates the breakdown of spent time between the `MPI_Start` and `MPI_Wait` calls in the pseudo-code. As a result, the offload version of persistent neighborhood *alltoall* collective implementation achieves $0.8\mu s$ in cost of `MPI_Start` and outperforms the existing MPI communications, such as MPI non-blocking point-to-point, persistent point-to-point, and non-blocking neighborhood collective, by a factor of two or more for short messages sizes (up to 16KiB).

1.3.2 Data Transfer Framework

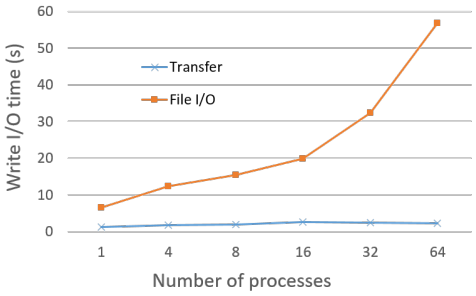
Multi-component workflows have become a common type of applications running in current HPC systems. Because the components are often developed independently, they are often coupled via files. However, file I/O becomes a bottleneck as the size of the data passed between components grows. To alleviate this problem, we developed a framework called Data Transfer Framework (DTF) that silently replaces file I/O with sending the data directly from one component to another over network[2]. The DTF assumes that the workflow components use PnetCDF for file I/O and uses the Message Passing Interface (MPI) library to send the data. Using the DTF, the developers of multi-component workflows can easily switch from file I/O to data sending without having to rewrite the I/O code.



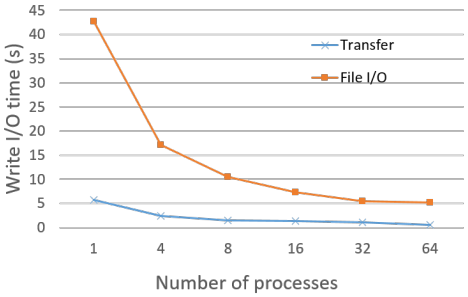
(a) BTIO: weak scalability test



(b) BTIO: strong scalability test



(c) S3D-IO: weak scalability test



(d) S3D-IO: strong scalability test

Figure 1.2: Time to perform data transfer

The main characteristics of the DTF are:

- Unlike many existing coupling solutions, the DTF requires only minimal modifications of the program and does not require modifications of PnetCDF I/O calls themselves;
- It automatically detects what data should be transferred to what processes transparently for the user, hence, it can be plugged into the workflow fast and with minimal efforts and there is no need to provide a description of the I/O pattern of the components;
- The DTF exhibits stable performance under different I/O loads.

The DTF comes in a form of a modified version of the PnetCDF-1.7.0 library and a library that provides a user API to enable the data transfer. The user must provide a simple configuration file that describes the file dependency in the workflow for the DTF.

The DTF intercepts PnetCDF calls in the program and handles them accordingly. If the PnetCDF read or write call was made for a file meant to be sent directly, instead of file I/O the call is transformed to a DTF *I/O request*. And the data transfer is performed via *the I/O request matching*. The matching consists of four steps. First, designated processes, called *master* processes, collect all read and write I/O requests for a given file. Then, each master finds out who holds the requested piece of data by matching each read request against one or several write requests. Finally, the master instructs the processes who have the data to send it to the corresponding process who requested it. The user must explicitly call a DTF API to invoke the I/O matching process.

In total there are three API user functions provided to the user:

- `dtf_init(config_file, component_name)` - initializes the DTF;
- `dtf_finalize()` - finalizes the DTF;
- `dtf_match_io(filename)` - invokes the I/O request matching for file *filename*;

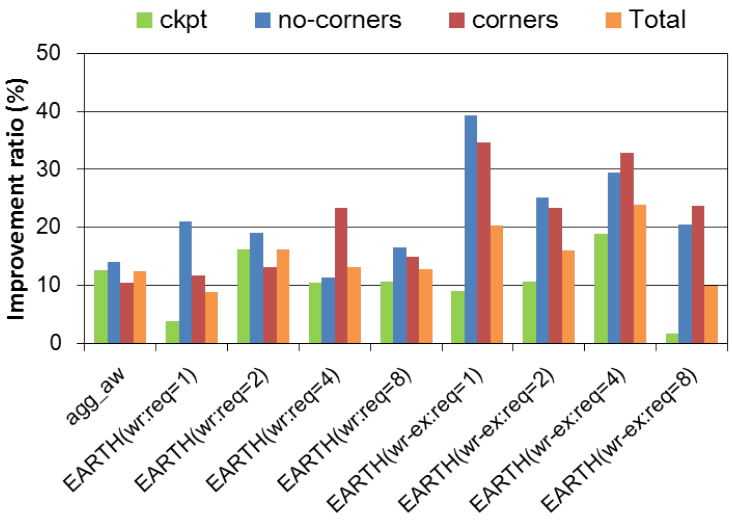


Figure 1.3: Performance improvements in FLASH-IO benchmark

All the API functions are collective, i.e. they should be invoked by all processes that share the file.

We demonstrate the performance of DTF on the K computer using two benchmark programs — BTIO and S3D-IO[1]. For each benchmark, we imitate a multi-component execution by running two instances of the benchmark: Processes of the first instance write to a shared file, processes in the second instance read from it. The I/O time is measured as the time between the moment the writer starts I/O matching and the moment when it receives a notification from the reader that it had got all the requested data. The results are presented on Figure 1.2. In the weak scalability test, the size of the shared file was adjusted in such a way depending on the number of processes so that each process transfers the same amount of data in each test: 800 MB for BTIO and 2 GB for S3D-IO. In the strong scalability test, the file size was fixed in all tests: around 12 GB for both S3D-IO and BTIO. As can be seen from the results, DTF shows a stable performance under different execution conditions.

1.3.3 Enhanced MPI-IO: EARTH

In FY2015, basic features of our enhanced MPI-IO library named EARTH(Effective Aggregation Rounds with Throttling) was built at the K computer. Effectiveness of I/O throttling and stepwise exchanges was already examined by using a very simple MPI-IO performance evaluation runs. In FY2016, we continued development of the EARTH to tune up its functions at the K computer, and tried performance evaluations with more application-oriented benchmarks. After some improvements, we measured performance of the EARTH using FLASH-IO benchmark. The benchmark code parallelized by MPI writes data blocks divided 3D data array with additional four guard cells in each dimension on both ends to hold information from neighbor processes. MPI-IO, PnetCDF, and HDF5 are supported in its write operation.

In this evaluation, we used HDF5 version 1.8.12 for the benchmark. we utilized the original MPI-IO of the K computer and the EARTH for an MPI-IO layer of HDF5 in order to examine performance improvements. We chose $32 \times 32 \times 64$ block sizes for 3,072 processes with the same number of compute nodes, thus we deployed one process per compute node. Figure 1.3 shows its write performance improvement ratios relative to the original MPI-IO. *ckpt* stands for improvement ratio in writing checkpoint files, while *no-corners* and *corners* represent improvement ratio in writing plot-files without corner data and writing corner data, respectively. *Total* denotes improvement ratio in total I/O time. *agg_aw* represents the EARTH with only aggregator layout optimization. While *EARTH* stands for the EARTH with I/O throttling, where numbers followed by *req* denote the number of I/O requests in throttling. Concerning the throttling cases, *wr* represents that only I/O throttling was used, while *wr-ex* stands for the case with both I/O throttling and cooperative stepwise data exchanges. Among the evaluated cases, *EARTH(wr-ex:req=1)* has showed the best performance, where we have achieved about 40% improvements in writing plot-file without corner data, and about 35% in writing plot-file for corner data. From the results, effectiveness of I/O throttling and stepwise data exchanges in the EARTH was confirmed.

[1] Available at http://cucis.ece.northwestern.edu/projects/PnetCDF/#Benchmarks

1.3.4 Sharing Virtual Address Space

Many core architectures become common in modern HPC and multi-process or multi-thread execution models are widely used on that architectures. Because the number of cores are increasing, researchers are keen to reduce the cost of communication among such large amount of executing processes or threads in a node.

In traditional multi-processes execution model, where each process is bound to a CPU core in HPC, the memory mapping technique is widely used to support communication between processes on a node, such as POSIX shmem and XPMEM. POSIX shmem, as its name suggests, is portable, but is not flexible to use in HPC runtime libraries, because it requires all involved processes. XPMEM is the other widely used memory mapping technique, which relies on kernel assistance. It dynamically exposes variables or data, but porting it onto non-Linux OS which commonly exists in HPC supercomputers (e.g., IBM BGQ, K) becomes hard. Moreover, the exposing / attaching cost is heavy, thus the runtime library developer has to carefully optimize to reduce overhead.

In the multi-thread execution model, the entire address space is shared thus the communication between threads can be more efficient than processes. However, porting the Virtual Address Space (VAS) sharing functionality of multi-threads into multi-processes execution model is not easy at all. Because maintaining the synchronization among threads in process-based applications or runtime systems can be extremely expensive because of lock contention and memory barriers (e.g., MPI). MPC is an efficient thread-based MPI implementation, thus allowing MPI processes to talk to each other as simple as threads. However, it heavily relies on special programming system including compiler, runtime library, and debugger.

There is a third memory sharing model, which gives the VAS sharing in multi-processes model without involving the complexity of threads. Such as SMARTMAP, PVAS[3-7]. However, all of those approaches requires change in kernel space, which is unpractical to use in large HPC environment.

In this fiscal year, we have succeeded to implement this third execution model completely at the user-level, and thus, it is portable and practical. This system is named “Process-in-Process” or “PiP” in short.

PiP is designed to be independent from OS kernels. Many high-end super computers are operated with dedicated operating systems. For example, the K computer runs with a specialized OS. If software depends on a specific OS kernel in any form, then the software loses its portability. XPMEM, for instance, is a Linux kernel module and unable to run on the K computer.

Table 1.1: PiP Portability

CPU	OS Kernel	Glibc version
Intel Xeon	Linux 3.10	2.17
Intel Xeon Phi (KNL)	Linux 3.10	2.17
	McKernel	2.17
AMD Opteron (ARM64)	Linux 4.2	2.17
the K computer and Fujitsu FX10 (SPARC64 IXfx)	XTCOS†	2.7

† Linux 2.6 based OS for the K computer and FX100

Another goal of PiP is language system independence. A typical language system consists of compiler, linker, runtime libraries, and debugger; it also may include profiling systems. None of thees is easy to develop. PiP is a small library of only about 3,000 lines and thus it is easy to maintain. Moreover, PiP is language independent. Indeed, Fortran programs and OpenMP programs run with PiP.

1.3.5 IHK/McKernel

This section summarizes recent development items of the IHK/McKernel lightweight multi-kernel operating system. We first provide a short introduction to the high-level architecture of the software stack and then discuss each particular new feature.

IHK/McKernel is a lightweight multi-kernel that comprises two main components: A low-level software infrastructure called Interface for Heterogeneous Kernels (IHK)[8] and an LWK called McKernel[9]. An architectural overview of IHK/McKernel is shown in Figure 1.4.

IHK provides capabilities for partitioning resources in a many-core environment (e.g., CPU cores and physical memory) and it enables management of LWKs. IHK can allocate and release host resources dynamically without rebooting the host machine. Additionally, IHK is implemented as a collection of kernel modules without any modifications to the Linux kernel code, which enables straightforward deployment on a wide range of Linux

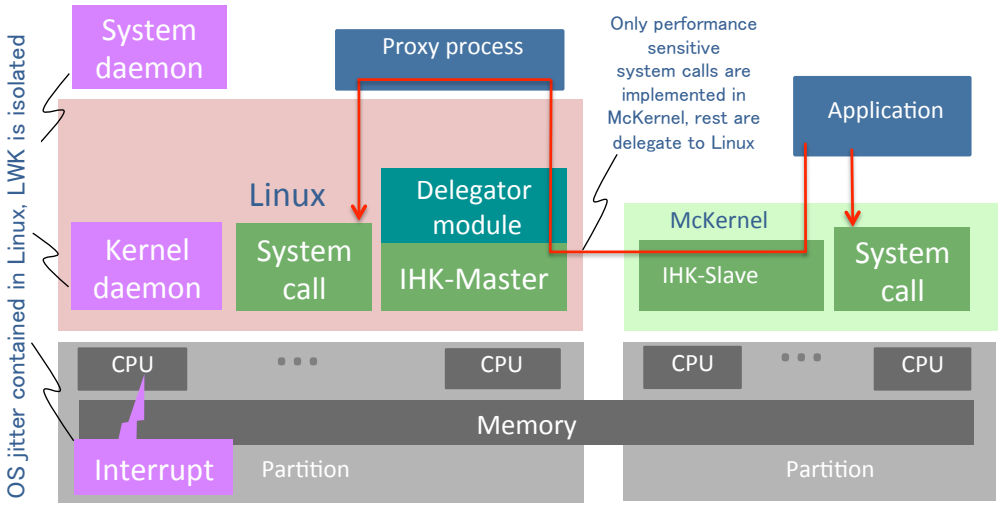


Figure 1.4: Overview of the IHK/McKernel architecture and the system call offloading mechanism.

distributions. Besides resource and LWK management, IHK also provides an Inter-Kernel Communication (IKC) layer, upon which system call offloading is implemented[8].

McKernel is an LWK developed from scratch. It is primarily designed for HPC and it boots only from IHK. McKernel retains a binary compatible ABI with Linux, however, it implements only a small set of performance sensitive system calls. The rest are offloaded to Linux. Specifically, McKernel provides its own memory management, it supports multi-processing and multi-threading, it has a simple scheduler, and it implements signaling. It also enables inter-process shared memory mappings and it provides standard interfaces to hardware performance counters.

For every single process running on McKernel there is a process spawned on Linux, called the *proxy process*. The proxy process' fundamental role is to facilitate system call offloading. It provides execution context on behalf of the application so that offloaded calls can be directly invoked in Linux. The proxy process also enables Linux to maintain various state information that would have to be otherwise managed by the LWK. McKernel for instance has no knowledge of file descriptors, but it simply returns the number it receives from the proxy process when a file is opened. The actual set of open files (i.e., file descriptor table, file positions, etc..) are tracked by the Linux kernel. We emphasize that IHK/McKernel runs HPC applications primarily on the LWK to achieve scalable execution but the full Linux API is available via system call offloading.

We have made a number of improvements to both IHK and McKernel throughout the past year. The followings summarize new features added to IHK:

- A topology aware IRQ routing framework has been developed to improve inter-kernel communication. Specifically, a mapping table defines for each LWK CPUs its target Linux CPU core. This enables balanced message delivery eliminating contention on internal message queue structures when multiple LWK CPUs interact with Linux simultaneously.

- IHK's memory reservation facility has been redesigned so that it can better handle fragmented Linux memory. Internally, a red-black tree data structure is utilized to reserve small contiguous blocks of physical memory which then recombined to larger blocks. Linux's page allocation API offers multiple page sized allocations (so-called compound pages). IHK's allocation algorithm starts from the largest possible allocations and it gradually decreases the compound page order to obtain smaller blocks. As a result, IHK can reliably reserve memory at the time LWK resources are requested.

Major McKernel improvements are as follows:

- Non-uniform memory (NUMA) is now fully supported by McKernel. This includes support for mainly two components. First, the correct exposure of topology information of the LWK partition via `/sys` and `/proc` filesystems. Second, LWK implementation of the NUMA related system calls, e.g., `get_mempolicy()`, `set_mempolicy()` and `mbind()`. As a result, McKernel supports standard Linux tools, such as `numactl` or `hwloc`.

- A redesigned, tree-based physical memory manager that provides better performance than McKernel's original bitmap based allocator.
- A number of HPC oriented features have been introduced which can be controlled by arguments to the `mcexec` command line tool. These include controlling heap extension, NUMA placement of BSS, DATA and TEXT segments, especially with regards of multiple memory types. Transparent utilization of large pages not only on heap, but also on BSS, DATA and stack segments. Optional disablement of `sched_yield()` when CPU cores are not oversubscribed, optional pre-mapping of shared memory segments to avoid page fault costs and the associated contention on internal kernel data structures. Pre-mapping stack segments. Bulk TLB remote invalidation to improve `munmap()` performance in multi-threaded applications.

1.4 Schedule and Future Plan

We continue to enhance performance and functionality of our system software stack for K, FX100, post-K, and other manycore architectures, such as Intel Xeon Phi.

1.5 Publications

1.5.1 Conference Papers

[1] Masayuki Hatanaka, Takahiro Ogura, Masamichi Takagi, Atsushi Hori, and Yutaka Ishikawa. Prototype implementation and evaluation of an mpi persistent neighborhood collective operation using tofu2 protocol offlaoding capability. In IPSJ SIG Technical Report, volume 2016-HPC-157, December 2016. (In Japanese).

[2] Tatiana Martsinkevich, Wei ken Liao, Balazs Gerofi, Yutaka Ishikawa, and Alok Choudhary. Improving multi-component application performance by silently replacing File i/o with direct data transfer: Preliminary results. In IPSJ SIG Technical Report, volume 2017-HPC-158. IPSJ, March 2017.

[3] Akio Shimada, Balazs Gerofi, Atsushi Hori, and Yutaka Ishikawa. Implementing Many-core Friendly MPI Intra-node Communication with New Task Model. IPSJ SIG Notes, (3), July 2012. (In Japanese).

[4] Akio Shimada, Balazs Gerofi, Atsushi Hori, and Yutaka Ishikawa. Pgas intra-node communication towards many-core architecture. In In PGAS 2012: 6th Conference on Partitioned Global Address Space Programing Model, PGAS'12, 2012.

[5] Akio Shimada, Balazs Gerofi, Atsushi Hori, and Yutaka Ishikawa. Proposing a new task model towards many-core architecture. In Proceedings of the First International Workshop on Many-core Embedded Systems, MES '13, pages 45-48, New York, NY, USA, 2013. ACM.

[6] Akio Shimada, Atsushi Hori, and Yutaka Ishikawa. Eliminating Costs for Crossing Process Boundary from MPI Intra-node Communication. In Proceedings of the 21st European MPI Users' Group Meeting, EuroMPI/ASIA'14, pages 119:119-119:120, New York, NY, USA, 2014. ACM.

[7] Akio Shimada, Atsushi Suto, Atsushi Hori, Yutaka Ishikawa, and Kenji Kono. Accelerating MPI Intra-node Communication Using Derived Data Types on Many-core. IPSJ-ACS, 9(2):46-63, July 2016. (In Japanese).

[8] Taku Shimosawa, Balazs Gerofi, Masamichi Takagi, Gou Naka- mura, Tomoki Shirasawa, Yuji Saeki, Masaaki Shimizu, Atsushi Hori, and Yutaka Ishikawa. Interface for Heterogeneous Kernels: BIBLIOGRAPHY 19 A framework to enable hybrid OS designs targeting high performance computing on manycore architectures.

[9] Balazs Gerofi, Akio Shimada, Atsushi Hori, and Yutaka Ishikawa. Partially separated page tables for efficient operating system assisted hierarchical memory management on heterogeneous architectures. In Cluster, Cloud and Grid Computing (CCGrid), 2013 13th IEEE/ACM International Symposium on, may 013.

Chapter 2

Programming Environment Research Team

2.1 Members

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Miwako Tsuji (Research Scientist)

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Christian Feld (Visiting Researcher)

Kengo Nakajima (Senior Visiting Researcher)

Tomoko Nakashima (Assistant)

2.2 Research Activities

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

In 2015FY, in order to archive these objectives above, we carried out the following researches:

(1) We continue working on the development and improvement of XcalableMP(XMP) programming languages. XcalableMP is a directive-based language extension, designed by XcalableMP Specification Working Group (XMP Spec WG) including some members from our team as a community effort in Japan. It allows users to develop parallel programs for distributed memory systems easily and to tune the performance by having minimal and simple notations. In this year, we have improved Coarray functions in Fortran for the K computer and others. In addition, benchmarks of Fiber miniapps are parallelized with XcalableMP and their performance is evaluated on the K computer.

(2) As an extension of XcalableMP to exascale computing, we are proposing a new programming model, XcalableACC, for emerging accelerator clusters, by integrating XcalableMP and OpenACC. We continue working on the language design and the compiler development of XcalableACC. This research is funded by JST CREST project on " post-petascale computing. In this year, we are get addtional fundings of SPPEXA project which is an international colloboration with French and Germany. Our goaln is to apply MUST verification tool to XMP for correctness checking of user applications.

(3) Co-design for HPC is a bidirectional approach, where a system would be designed on demand from applications, and applications must be optimized to the system. We started the design of tools for co-design, including the SCAMP profiler for the network of large scale systems.

(4) As the post-K computer will be a large-scale multicore-based system,we are investigating programming models for manycore-based parallel systems as a next version of XcalableMP, especially for the integration of dynamic tasking with PGAS programming model.

(5) We conducted several collaborations on the performance evaluation with JSC, University of Tsukuba, Kyusyu Institute of Technology and other groups. In the collaborations with Kyusyu Institute of Technology, a task parallel language Tascell was evaluated on the K computer. As for performance tuning tools, We continue the collaboration with JSC for g a tuning tool Scalasca, which is being developed by JSC, for the K computer.

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

- XcalableMP workshop (Nov. 11)
- FOCUS tutorial on XMP (April 21, Dec. 8)

The seminar or tutorials consist of both classroom and hands-on learning

2.3 Research Results and Achievements

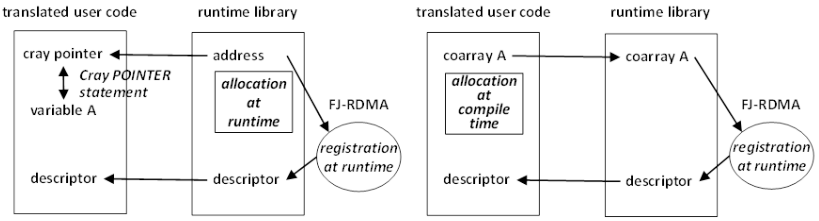
2.3.1 Enhancement of Omni XcalableMP CAF translator

We are developing Omni XcalableMP that is an open-source XcalableMP compiler, in cooperation with the university of Tsukuba. The latest version 1.0 has been released in November, 2016

Coarray Fortran (CAF) is a successful Partitioned Global Address Space (PGAS) language, which is now a part of Fortran 2008 standard [1]. We have been developing Omni CAF compiler [2], which is a part of Omni XcalableMP (XMP) compiler, and achieved higher performance than other implementations, UH-CAF in U. of Houston, OpenCoarrays and Intel Fortran. A reason of such high performance is that only our compiler is a source-to-source compiler and can work together with a sophisticated Fortran compiler chosen as the backend. Therefore, we think it is important to extract higher performance from the backend compiler to get the performance of our compiler higher.

Omni XMP CAF compiler has achieved as high performance as MPI in some highly-tuned benchmark codes. According to the performance result of CAF versions of NASParallel CG program, the "highly-tuned" version was 0.2% to 5.8% faster than the MPI version. The next issue was that the "tuned" version, which was not highly but fairly tuned, got only 22% to 59% of the performance of the MPI version. The reason of the low performance was performance drop of the computation part comparing with serial version of the same program.

After detailed analysis, we found that the coarray variables look as pointer variables in the "tuned" version and as non-pointer dummy arguments in the "highly-tuned" version from the viewpoint of the backend compiler.



(a) RA/RR method (b) CA/RR method

Figure 2.1: Memory allocation systems for coarray variables

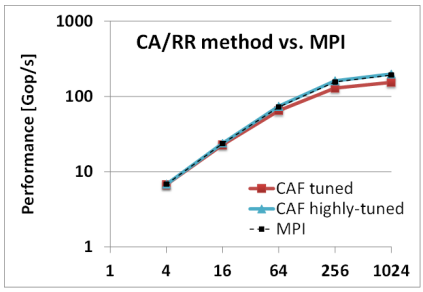


Figure 2.2: Result of NPB CG using CA/RR method

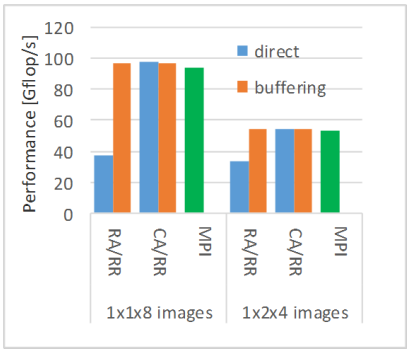


Figure 2.3: Comparison on Himeno benchmark: RA/RR and CA/RR, MPI

Pointer variables appearing in the computation loops often suppress such compiler optimizations as prefetching, software pipelining, SIMD vectorization and automatic thread parallelization. Omni CAF translator should prevent converting the coarray variables to pointer variables as much as possible.

In addition to the previous implementation of the memory management of coarrays, we have implemented a new algorithm to avoid generating pointer variables. The former, called RA/RR (Runtime Allocation/Runtime Registration) method, both allocates and registers coarrays in the runtime library. The provided address is passed to the address of the coarray variable, which looks as a pointer from the viewpoint of the Fortran compiler. The latter, called CA/RR (Compile-time Allocation/Runtime Registration) method, allocates coarrays by the Fortran system, and the address is passed to the Fujitsu "low-level communication library" FJ-RDMA to be registered.

Figure 2.1 illustrates RA/RR and CA/RR methods. In (a) the RA/RR method, the runtime library allocates the data object and shares the address with the user code that is translated by the CAF translator. The user code regards this address as the address of the coarray due to the Cray pointer mechanism. In (b) the CA/RR method, the coarray is declared as a usual common variable in the user code and is passed to the runtime library. In both cases, the address and other information of the coarray is registered with the communication library FJ-RDMA and as the result the descriptor is passed to the output code.

Figure 2.2 shows the result of CA/RR method on NAS Pareallel CG. The performance of the "tuned" version of CAF code is clearly improved and 80% to 99% performance of MPI version.

Figure 2.3 compares the RA/RR and CA/RR methods using the Himeno benchmark. Two versions of CAF code were ported from MPI code; in version "direct", the main variable appearing in the Jacobi calculation loop is declared as a coarray, and, in version "buffering", only buffer variables are declared as coarrays, which do not appear in the computation part. The figure shows CA/RR method provides high performance even in version "direct" while RA/RR method drops in the performance. The version "direct" of Himeno with 8 images performs 37 Gflop/s in RA/RR and 98 Gflop/s in CA/RR. It can be said that the existence of pointer variables seriously disturbs the compiler optimization and avoiding it is very effective to improve the total performance.

2.3.2 Coarray-based Implementation of Fiber Miniapp Suite using XcalableMP

Fiber is a miniapp suite that is maintained primarily by RIKEN AICS for next-generation supercomputing. Fiber consists of 8 minapps: CCS (QCD lattice QCD), FFVC-MINI(Navier-Stokes solver for 3D unsteady thermal flow of incompressible fluid), NICAM-DC (nonhydrostatic icosahedral atmospheric model) mVMC-MINI(analysis of the physical characteristics of the strongly correlated electron systems), NGS Analyzer-MINI (human genome analysis to identify genetic differences among persons or cancer cell's mutation), MODYLAS-MINI(general-purpose molecular dynamics simulation), NTChem-MINI(molecular electronic structure calculation), FFB-MINI(general-purpose thermal flow FEM program). Each miniapp in Fiber is parallelized with MPI; in addition, some are explicitly multithreaded with OpenMP.

The goal of this study is to implement Fiber using XcalableMP(XMP) language and to evaluate the productivity and performance of XMP. One of the remarkable characteristics of XMP is that it supports both global-view and local-view parallelization. As a first step, we carried out the implementation and evaluation of local-view parallelization using coarray.

To obtain a coarray-based implementation, MPI communication functions in each miniapp must be replaced with their corresponding coarray notations; this is based on the following rules. Note that the rules beloware based on remote writes (puts), but the rules can also be based on remote reads (gets).

- MPI_Send & MPI_Isend ⇒ assignment statement with a coarray on the left-hand side
- MPI_Recv & MPI_Irecv ⇒ to be removed
- collective communication ⇒ intrinsic subroutine of Fortran 2015 such as co_broadcast and co_sum
- MPI_Wait & MPI_Barrier ⇒ sync all statement

Some collective communication functions, such as MPI_Allgather, that have no available corresponding intrinsic subroutines available should be replaced with a set of coarray assignment statements corresponding to the send/recv pairs extracted from their communication pattern.We adopt the above very simple rules for the preliminary implementation in this study. Note that some optimizations (e.g. deleting redundant sync all statements) can be applied for higher efficiency.

In general, for one-sided communication including coarray assignments, the process that invokes communication (origin) is required to know information about the buffer on the other side (target) with which it interacts. Therefore, for irregular communication (e.g. halo exchange for unstructured meshes), processes must exchange buffer information with each other in advance of actual communication; such information is trivial for regular communication and not needed for two-sided communication. In the Fiber miniapp FFB-MINI, because a process receives data from multiple sources and the size of data received from each source is determined at runtime, the data are packed into a receive buffer while incrementing the displacement.

We implemented five miniapps (CCS QCD, NICAM-DC, MODYLAS-MINI, NTChem-MINI, and FFB-MINI) of the Fiber miniapp suite using the coarray feature of the XMP PGAS language.These are regular miniapps and were rewritten by replacing MPI communication functions with coarray notations on the basis of simple rules. However, for irregular miniapps such as FFB-MINI, more complicated rewrites were needed because a node or image must exchange information about its own communication buffers with each other in advance of actual data movement.

We evaluated the coarray-based implementation of the five miniapps (CCS-QCD, NICAM-DC,MODYLAS-MINI,NTChem-MINI, and FFB- MINI) from Fiber on the K computer. The performance of the original MPI version was also evaluated for comparison. The coarray feature of Omni XMP is based on the the extended RDMA interface dedicated to the K computer. Figures 2.4 and 2.5 shows the results of CCS QCD and NICAM-DC, respectively. The evaluation showed that our coarray-based implementations of three (NICAM-DC, NTChem-MINI, and FFB-MINI) of the five miniapps were comparable to their original MPI implementations. However, for the remaining two miniapps (CCS QCD and MODYLAS-MINI), there was performance degradation, which was due to the large overhead of allocating dynamic coarrays.

2.3.3 Fault tolerant features in a multi-SPMD programming model

Supercomputers in the exa-scale era would consist of a huge number of nodes arranged in a multi-level hierarchy. In order to exploit the full performance of such systems, we had been proposed a multi SPMD programming model, which use multiple programming models across different architectural levels and had been developed a software to realize the proposed programming model by adopting a scientific workflow environment and a PGAS

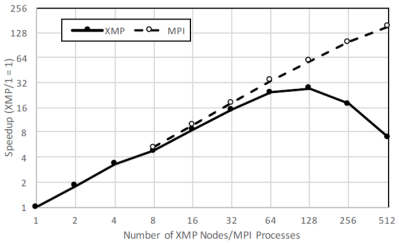


Figure 2.4: Result of CCS QCD

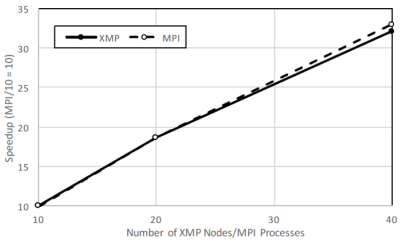


Figure 2.5: Result of NICAM-DC

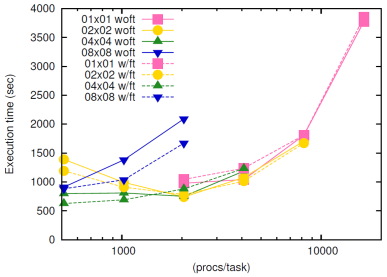


Figure 2.6: Overhead of the heartbeat messages

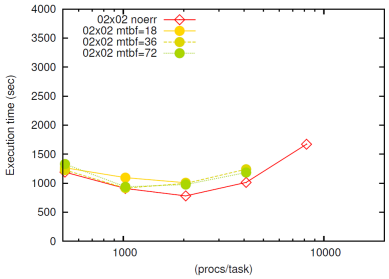


Figure 2.7: Execution time under different expected MTBFs

language called XcalableMP (XMP). In 2016, we extend the program model to realize fault tolerance without any modification in application-source-code and performed experiments in the K computer.

We have introduced heart beat messages into our middleware and modified scheduling model in the workflow scheduler. According to the experiments, the overhead of heart beat messages to detect errors seems to be ignorable. However, in the K computer, we found that the data import/export to/from tasks using MPI-IO functions sometimes disturb the heart beat messages sent by task programs. Therefore, we have introduced a new mechanism to solve the issue, which send a special heart beat message to inform the start of MPI-IO. Other experiments we have performed suggested that the best way to exploit the hieratical parallelism in the multi-SPMD programming model should be changed under different assumed mean time between failures (MTBFs)
.

2.3.4 OpenMP Extension for Explicit Task Allocation on NUMA Architecture

Most modern HPC systems consist of a number of cores grouped into multiple NUMA nodes. The latest Intel processors have multiple NUMA nodes inside a chip. Task parallelism using OpenMP dependent tasks is a promising programming model for many-core architecture because it can exploit parallelism in irregular applications with fine-grain synchronization. However, the current specification lacks functionality to improve data locality in task parallelism.

We propose an extension for the OpenMP task construct to specify the location of tasks to exploit the locality in an explicit manner.

Figure 2.8 shows the conceptual model of our approach. The software system consists of multiple task queues connected to each NUMA node respectively. Assume that an application generates a number of OpenMP task which carries out computations on a single element of array A. The figure shows how tasks and data can be allocated on NUMA nodes and matched with the help of information given by the programmer.

First, the programmer distributes the array among NUMA nodes by using existing NUMA libraries such as libnuma. Then the programmer describes OpenMP tasks with a hint about which element would be accessed in the task. The node_bind clause used in the task construct, which we propose in this paper, gives the information to the OpenMP compiler and runtime. The OpenMP compiler can determine the node id that the specified element is allocated. The OpenMP runtime utilizes it to schedule the task to the corresponding task queue. In our implementation, a group of cores connected to the same NUMA node has a higher priority to access the corresponding task queue than others so that the cores would have more chance to access the local memory. This

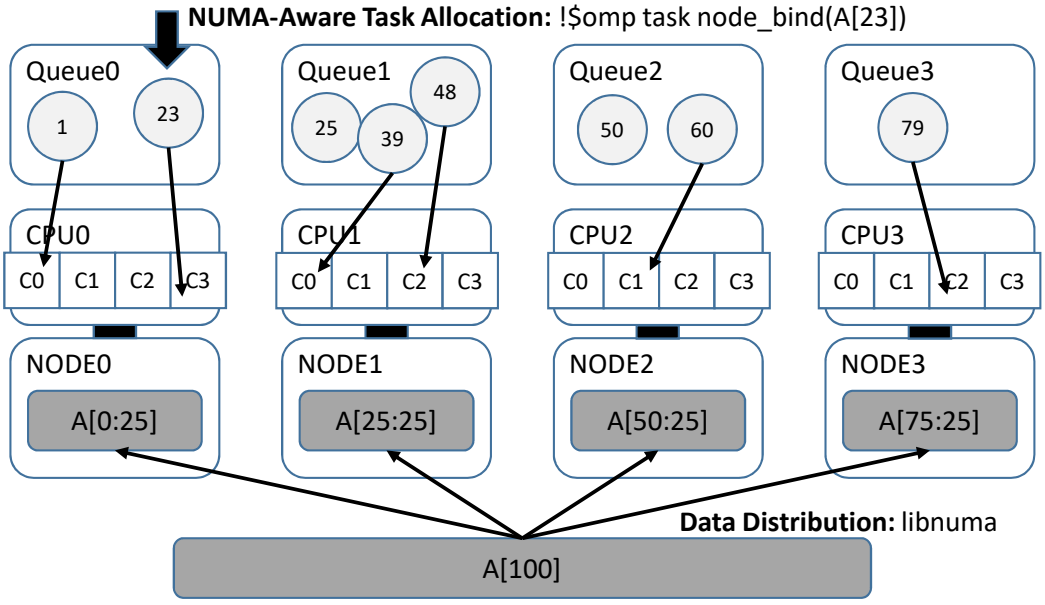


Figure 2.8: NUMA-Aware Data Distribution and Task Allocation

approach provides an explicit way of improving data locality in tasks by combining explicit data distribution.

The node_bind is defined as an additional clause to the task construct. It takes one variable reference that its address can be determined by the compiler. The compiler assigns the target task on the same node that the specified variable is allocated. The following shows an example code of the node_bind clause. The code is taken from the Strassen kernel in KASTORS. The output array C is given in the node_bind clause. When M2 and C are allocated on the same NUMA node, the task can be executed without any remote memory access.

```
#pragma omp task depend(inout: C) depend(in: M2) \
            private(Row, Column) node_bind(C[0])
for (Row = 0; Row < QuadrantSize; Row++)
  for (Column = 0; Column < QuadrantSize; Column += 1)
    C[RowWidthC*Row+Column] += M2[Row*QuadrantSize+Column];
```

We have implemented the node_bind clause modifying GNU Compiler Collection (GCC) version 5.3.0. GCC 5.3.0 supports OpenMP 4.0 features including the task depend clause. We measured the performance of the KASTORS benchmark kernels using GCC and our implementation. Our evaluation platform is Intel Xeon CPU E5-2699 v3, 2 sockets, 2.3GHz, COD enabled: Each CPU has 18 physical cores and 2 NUMA nodes (when the COD mode is enabled).

Figure 2.9 shows the performance speedup of the Jacobi kernel against the serial version. The matrix size is 16384 x 16384 and the block size is 1024. The original FOR, TASK, and TASK DEP version (*task init* and original in Figure 2.9) initializes the grid point values in parallel execution of independent tasks so that the memory pages are distributed among NUMA nodes in a random manner. On the other hand, the modified TASK and TASK DEP version initializes the grid points using loop work sharing in a parallel region. As a result, the memory pages are evenly distributed among nodes.

The performance of the FOR version shows that the initialization scheme can change the performance. Compared with *for init*, the FOR version initialized using the parallel for construct, *task init* achieves the lower performance than *for init* because the memory pages are allocated randomly among NUMA nodes. *for init* achieves the best performance because the access pattern of the initialization and the computation is perfectly matched.

The modified TASK and TASK DEP version achieve better performance than the original versions for the same reason of *for init*. It reduces remote page access by matching the data afgllocation pattern and the task

scheduling pattern. The reason why the TASK version show the lower scalability than the TASK DEP version is that there is a global synchronization (taskwait construct) between the update phase and the computation phase.

2.4 Schedule and Future Plan

We have been developing a production-level XcalableMP compiler and make it available for the K computer's users as well as the users of conventional clusters. The specification of XcalableMP is designed and examined by XcalableMP Specification Working Group. While so far the version of the spec is version 1, we concluded that a set of spec in version 1 is now "converged"? and new functions should be discussed for version 2. The important topics for XcalableMP 2.0 might include the support for manycore clusters, that is multitasking with integrations of PGAS model. We are now working on the study of the programming models for post-petascale, including programming models and runtime techniques to support manycore.

Towards exascale computing, there are two major approaches, manycore and GPU. We are already working on XcableACC as a solution for accelerator-based system, which is to be explored in the JST CREST project, and will develop it for a new type of accelerator such as FPGA.

The post-K system is supposed to take the manycore approach. Manycore system has not only a plenty of cores, but also each core may support wide-length SIMD unit. We are interested in the optimization for SIMD, and the API to tell the compiler how to optimize the code using SIMD. We are now investigating several techniques for these purpose using an open compiler infrastructure LLVM and Omni Compiler Infrastructure.

2.5 Publications

2.5.1 Journal Articles

[1] Keisuke Tsugane, Taisuke Boku, Hitoshi Murai, Mitsuhisa Sato, William M. Tang, Bei Wang, "Hybrid-view programming of nuclear fusion simulation code in the PGAS parallel programming language XcalableMP." Parallel Computing 57: 37-51 (2016)

[2] Masahiro Nakao, Hitoshi Murai, Hidetoshi Iwashita, Taisuke Boku, Mitsuhisa Sato."Implementation and evaluation of the HPC Challenge benchmark in the XcalableMP PGAS language," International Journal of High Performance Computing Applications, Mar. 2017. doi: 10.1177/1094342017698214.

2.5.2 Conference Papers

[3] Jinpil Lee, Keisuke Tsugane, Hitoshi Murai, Mitsuhisa Sato."OpenMP Extension for Explicit Task Allocation on NUMA Architecture," 12th International Workshop on OpenMP, Nara, Japan, Oct. 2016.

2.5.3 Invited Talks

[4] Mitsuhisa Sato, "Challenges for Parallel Programming Models and Languages of post-petascale and exascale computing – Status of Flagship 2020 'Post-K' project", CCP, July 2016.

[5] Yutaka Ishikawa and Mitsuhisa Sato, "Development of system software in post K supercomputer", 12th International Workshop on OpenMP, Nara, Japan, Oct. 2016.

[6] Mitsuhisa Sato, "FLAGSHIP 2020 project : Challenges for post-petascale and exascale Computing," SC16 HPC Connection WS, Nov, 2016

[7] Mitsuhisa Sato,"FLAGSHIP 2020 project: Development of 'post-K' and ARM SVE", The second annual Arm HPC User group at SC16. Nov. 2016.

2.5.4 Posters and Presentations

[8] Hitoshi Murai, Taisuke Boku, Matthias S. Muller, Christian Terboven, Joachim Protze, Pablo Reble, Serge G. Petiton, Nahid Emad. "MYX: MUST Correctness Checking for YML & XMP Programs," ISC16/HPCAsia Poster, Frankfurt, Germany, Jun. 2016.

[9] Miwako Tsuji, Jinpil Lee, Taisuke Boku, Mitsuhisa Sato. “SCAMP: ’Pseudo’ Trace Driven Simulation toward Scalable Network Evaluation,” ISC16/HPCAsia Poster, Frankfurt, Germany, Jun. 2016.

[10] Jinpil Lee, Tsugane Keisuke, Daisuke Sugiyama, Murai Hitoshi, Mitsuhisa Sato. “Tasklet: Multitasking in a PGAS Language for Many-Core Clusters,” ISC16/HPCAsia Poster, Frankfurt, Germany, Jun. 2016.

[11] Mitsuhisa Sato, Hitoshi Murai, Masahiro Nakao, Hidetoshi Iwashita, Jinpil Lee, Akihiro Tabuchi. “Omni Compiler and XcodeML: An Infrastructure for Source-to-Source Transformation,” Platform for Advanced Scientific Computing Conference (PASC16), Lausanne, Switzerland, Jun. 2016.

2.5.5 Patents and Deliverables

[12] Omni XcalableMP compiler ver. 1.0 (registered as an AICS-supported software)

Chapter 3

Large-Scale Parallel Numerical Computing Technology Research Team

3.1 Members

Toshiyuki Imamura (Team Leader)

Yiyu Tan (Researcher)

Yoshiharu Ohi (PostDoctoral Researcher)

Yusuke Hirota (PostDoctoral Researcher)

Daichi Mukunoki (PostDoctoral Researcher)

Daisuke Takahashi (Senior Visiting Researcher)

Franz Franchetti (Visiting Researcher)

Yoshio Okamoto (Visiting Researcher)

Takeshi Fukaya (Visiting Researcher)

Shigeo Orii (Research Consult)

Doru Adrian Thom Popovich (Student Trainee)

Masaaki Aoki (Student Trainee)

Masatoshi Takayanagi (Student Trainee)

Ryota Kayanuma (Student Trainee)

Koichiro Watanabe (Student Trainee)

Yukiko Akinaga (Assistant)

Aya Motohashi (Assistant)

3.2 Research Activities

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

precision, resiliency, and scalability. Our primary mission is to develop and deploy highly parallelized and scalable numerical software on K computer, namely KMATHLIB. It comprises several components such as for solving

- systems of linear equations,
- eigenvalue problems,
- singular value decomposition,
- fast Fourier transforms, and
- nonlinear equations.

The K-specific topics and technical matters for emerging supercomputer systems are also our challenging works such as

- Tofu interconnect,
- parallel I/O,
- fault detection (soft-error), and
- higher accuracy computing.

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

3.3 Research Results and Achievements

ollowing series of the annual reports from 2012-13 to 2015-16, we summarize the latest results of our running projects, mainly focused on 1) development of KMATHLIB, 2) development of EigenExa, 3) investigation of FDTD related methods, and 4) other fundamental studies to optimize the BLAS kernels through automatic parameter tuning. The plans and the publication list are also presented in the last section.

3.3.1 Extension of Usability and Maintainability for Numerical Libraries

3.3.1.1 KMATHLIB_API

KMATHLIB_API is a software framework to use numerical libraries via uniform interfaces, and includes large-scale, highly parallel and high-performance numerical libraries and related software for peta-scale supercomputer systems such as the K computer. Since the data structures and the usage of the numerical libraries are generally different, we must understand them to use the numerical libraries. If some numerical libraries are used in a program, data structure conversion is often necessary. Therefore, a program becomes complicated, and the cost of application development and the maintenance increase. If KMATHLIB_API is used, the data structure conversion such as the above is automatically treated by internal functions of KMATHLIB_API. KMATHLIB_API provides highly abstracted interfaces, and various numerical libraries are available by the uniform description of the program. The software package of KMATHLIB_API was released in May 2016. Accordingly, we promoted KMATHLIB at the poster session in JSIAM 2016 [29]. Also, we continue to develop about a framework function improvement of KMATHLIB_API. For the partial support from COE program, we made the tutorial materials of KMATHBLI_API, and held the lecture class of AICS public software 'KMATHLIB' using such materials on 28th March 2017.

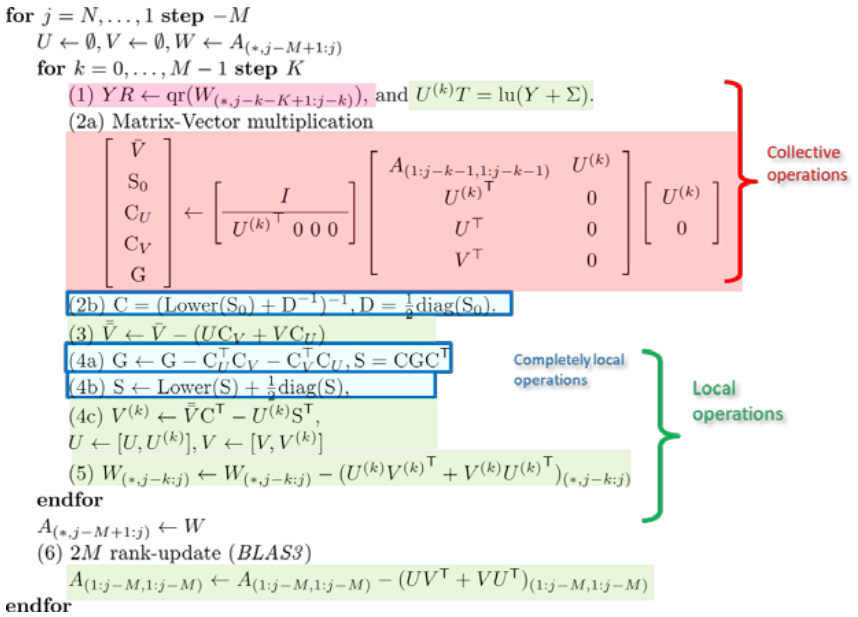


Figure 3.1: Block CAHTR algorithm

3.3.2 Performance Optimization by Communication Avoidance and Communication Reduction

3.3.2.1 Performance Modeling by Overfitting with Non-Negative Constraints

In order to establish a methodology for the performance prediction model for large-scale parallel computing, the LP method, which introduces suppress of overfitting with non-negative constraint, is applied to predictive models of HPL running on an SGI ICE X and EigenExa running on the K computer [9]. In previous works, we examined that the LP method predicted more accurately than the lasso's method, which is often used in the sparse modeling field. We selected the base functions as $\{N^3, N^2, N, N^3/\sqrt{p}, N^2/\sqrt{p}, N/\sqrt{p}, N^3/p, N^2/p, N/p\}$, and constructed a model functions represented by a linear combination of the base functions. The obtained model of EigenExa presents communication cost, especially the sum of `MPI_Allreduce` and `MPI_Bcast`, as

$$c_1 \frac{N^2}{\sqrt{p}} + c_2 N^3 + c_3 N.$$

The result contains unexpected factors N^3, which does not come from theoretical discussions and has no effect of parallelization. Then, it suggests that a large scale eigenvalue problem incurs performance degradation due to communication overhead.

3.3.2.2 Block-CAHTR

Communication avoidance (CA) is considered to be a promising technology to overcome the drawbacks resulting from the communication latency. We proposed CAHTR (CA-Householder TRidiagonalization) method in FY2015-16. The algorithm performs effectively on the expected situations such as computing a small problem with a number of processes. We have extended CAHTR as a block algorithm, which naturally improves parallelism and reduces communication latency.

In Fig 3.1, the statements highlighted in red require three `MPI_Allreduce`'s per iteration. The proposed algorithm was presented at PMAA2016 conference [19], and overview of our research activities for Communication Avoidance (CA) and Communication Hiding (CH) technique was presented at SIAM CSE2017 [24].

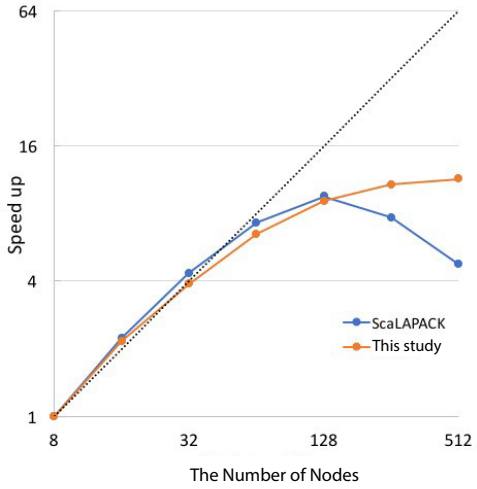


Figure 3.2: Strong scaling (Speed up) for CAQR method on K computer.

3.3.2.3 Communication Avoiding QR

We have studied Communication Avoiding QR factorization (CAQR). Needless to say, QR factorization is a significant algorithm in a large scale matrix decomposition, and it is taken advantage in the least square approximation, orthogonalization of vectors, singular value decomposition (SVD), and computing a Moor-Pennrose pseudo-inversion, et al. At the moment, ScaLAPACK is thought as a de facto standard numerical package for QR factorization on distributed parallel computers. However, it does not perform on modern multicore cluster systems, efficiently. We introduced a tiling CAQR algorithm, in which a tiling method and CAQR are combined. The algorithm is suitable for massively parallel computing because it reduces communication overhead radically. Our implementation shows better performance improvement than ScaLAPACK when the number of nodes is beyond a couple of hundreds (see Fig. 3.2).

3.3.3 More Advanced Implementation of Eigenvalue Solver

3.3.3.1 Performance Evaluation of a Quadruple Precision Eigenvalue Solver QPEigenK/QPEigenG

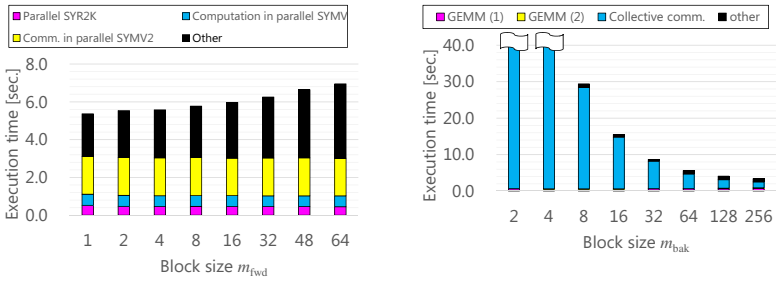
We have been studying on quadruple precision eigensolvers in collaboration with Japan Atomic Energy Agency. In many computational science and engineering applications, large and dense eigenvalue problems are frequently solved. As the matrix dimension increases, the accuracy of the computed eigenpairs generally becomes worse due to rounding error. Therefore, higher precision eigensolvers are required in some of the applications. However, at the start of FY2016, only double precision eigensolvers (such as PDSYEVD, PDSYGVD routines in ScaLAPACK) were available for massively parallel distributed memory parallel computers (e.g. the K computer). To overcome the problem, JAEA and we have developed a quadruple precision standard and generalized eigensolver libraries QPEigenK and QPEigenG, respectively. Based on a double precision eigensolver library EigenK, JAEA has implemented the eigensolvers of QPEigenK and QPEigenG, in which all the computations are carried out in double-double arithmetic. We have evaluated and analyzed the performance of the solvers.

We measured execution time for a various number of block sizes on the K computer. We observed that the eigensolvers in QPEigenK and QPEigenG show an excellent scalability on the K computer. The results were presented in HPC in Asia Poster Session held with an international conference ISC'16 [10].

We also carried out an analysis of the performance of the eigensolvers in QPEigenK with a performance improved quadruple precision BLAS on the K computer. We found that the increase of the block size does not accelerate the tridiagonalization (Fig. 3.3a) while it reduces the time for back transformation (Fig. 3.3b). The results were presented at international conferences [15,17] and a domestic conference [25].

3.3.3.2 Divide-and-Conquer Algorithm for Manycore Systems

Recent manycore processors (e.g. Intel Xeon Phi Knights Corner (KNC) and Knights Landing) have significantly high FLOPS. However, to run applications efficiently on the manycore systems, it is required to fully utilize a



(a) Tridiagonalization (b) Back transformation

Figure 3.3: Execution time of tridiagonalization and back transformation for various block sizes ($n = 5000$, 512 nodes).

large number of threads and cores of the processors. The de facto standard tridiagonal eigensolver DSTEDC in LAPACK is based on a divide-and-conquer algorithm for a sequential environment. In the solver, the tree parallelism of the divide-and-conquer method is not exploited at all. Thus, it can be expected that DSTEDC does not work efficiently on manycore systems.

We proposed a parallel divide-and-conquer algorithm based on a new execution scheduling by batched kernels on manycore system. In the proposed algorithm, the procedures of the merges in a layer are grouped by kind. The grouped procedures have sufficient parallelism, moreover, they are carried out by parallelized batched kernels. In addition, the use of vendor provided optimized kernels (e.g. batched DGEMM) for the grouped procedures leads further speedup. Thus, it can be expected that the proposed algorithm works efficiently in a highly parallel environment.

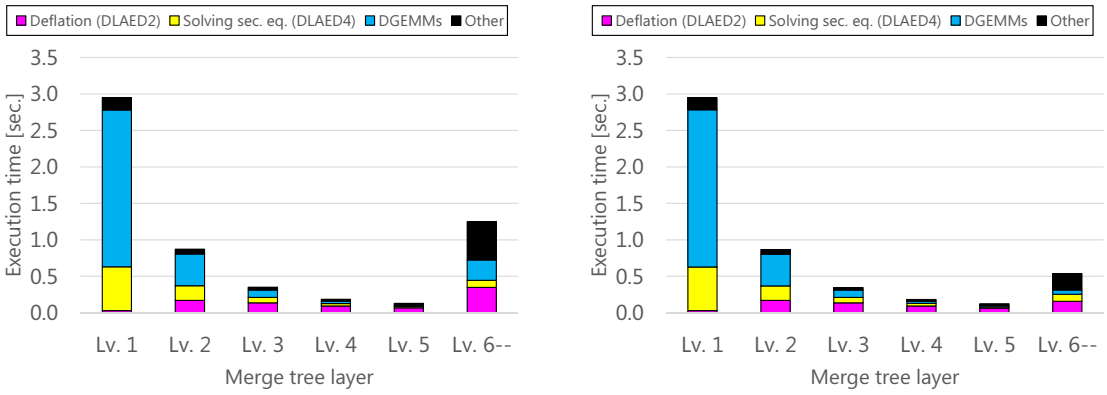
We evaluated the execution time and its breakdown of the implementations based on the conventional and proposed algorithms on Xeon Phi KNC 3120P. Due to technical reasons, the implementation based on proposed algorithm is only partly optimized. From the results of numerical experiments, we observe that the implementation of the conventional algorithm takes a long time for the low layers of the merge tree (Fig. 3.4a). On the other hand, the execution time of the implementation based on our program for the low layers and other layers are much shorter than and comparable to the implementation based on the conventional algorithm, respectively (Fig. 3.4b). As a whole, the implementation based on our algorithm is about 15% faster than the conventional one while the implementation based on our algorithm is not well optimized. The results were presented in [16] and [6].

3.3.4 Development of High-Performance Linear Algebra Libraries on Future Architectures

In recent years, the improvement of single processor performance has reached its technological limits, and the improvement of system performance has to rely on increasing parallelism. In fact, the number of processors in a system, the number of cores in a processor, and the vector length of SIMD processors are increasing. As computer architecture becomes more complex and more parallelized, software development and code optimization will be made more challenging. Also, not only to achieve high performance, but also to support accurate, fault-tolerant, and energy-efficient computations are required toward the emerging exascale computing. Therefore, we are conducting a study for developing linear algebra software with a new design on modern many-core architectures such as GPUs and highly parallel systems.

3.3.4.1 Automatic Thread-Block Size Adjustment for Memory-Bound BLAS Kernels on GPUs

We have been studying the implementation and optimization techniques of linear algebra kernels such as BLAS on GPUs for a few years. In the previous FY, we proposed a method to determine the nearly optimal thread-block size on memory-bound BLAS kernels on GPUs. It is known that the performance of CUDA kernels often



(a) Conventional algorithm

(b) Proposed algorithm

Figure 3.4: Execution time breakdown of implementations by merge tree layers ($n = 12000$)

depends on the number of threads per thread-block (thread-block size), and the optimal thread-block size often differs according to the GPU hardware running the kernel and the given data size to the kernel. Therefore, such a method to determine the optimal thread-block size is required to develop high performance CUDA kernels. In this FY, we submitted a paper about the method to an international conference and had a presentation (ATMG 2016 [5]). The results were introduced and discussed in some other conferences (poster presentation at GTC Japan 2016 [28], oral presentation at ATμWS2016 [27] and SIAM CSE17 [22]).

3.3.4.2 Reduced-Precision Floating-Point Formats

In FY2015, we proposed the implementation of reduced-precision floating-point formats that have shorter significand bit-length than IEEE standards on GPU and CPU. By eliminating waste data movement in the computation using such reduced-precision formats, we expect to save memory (cache) usage and improve the computation speed and energy efficiency. In this FY, we continued the study and had a poster presentation at an international conference (poster presentation at Cluster 2016 [11] with extended abstract). In this presentation, we showed the performance of our reduced-precision formats on some linear algebra kernels including sparse matrix-vector multiplication on three GPUs. We introduced the results in a domestic event (poster presentation at GTC Japan 2016 [28]) and a domestic workshop (oral presentation at LSPANC2017 [21]) as well.

3.3.4.3 Verified Computation for Linear Systems on Supercomputers

Although most numerical computations are performed with floating-point operations, the precision is limited, and the computation results may have errors due to rounding. Therefore, the result of floating-point operations is just an approximate solution of the problem, and in general, we are not able to know how accurate the solution is. Verified computation is a technique to give the accuracy of the approximate solution obtained by floating-point operations. However, the performance of verified computations on highly parallel computers has not been well discussed so far. We evaluated the performance of a program of the verified computation for solving linear systems $Ax = b$, developed by Dr. Morikura et al. at Waseda University, on the K computer and the FX100 system installed in RIKEN ACCC. The theoretical cost of the verified computation takes six times of that without verification (approximate computation using general floating-point operations). However, we showed that when the number of nodes is increased for a fixed size problem, the actual cost of the execution time can be about two times of that due to the difference of the performances in terms of strong-scaling. This result was presented at an international conference (oral presentation at EASIAM 2016 [4]) and a domestic

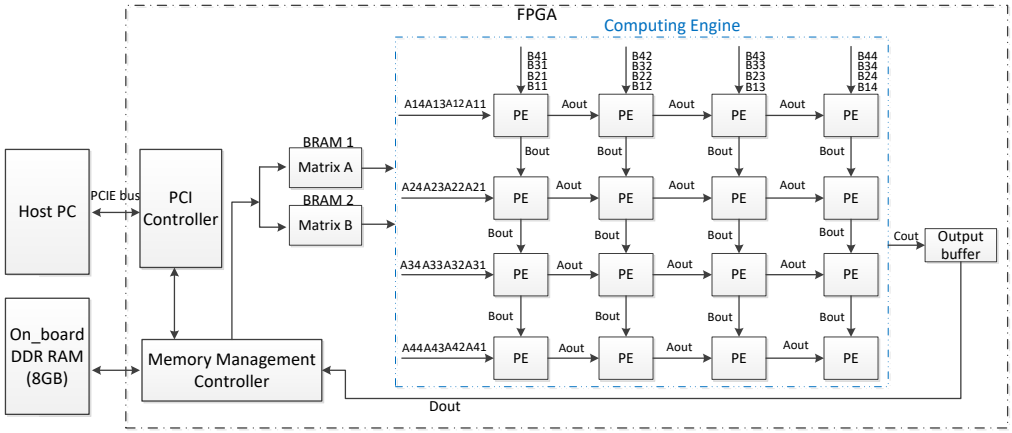


Figure 3.5: FPGA diagram for Matrix-matrix multiplication

workshop (oral presentation at HPC157 [8] with technical report).

3.3.5 Hardware-based Acceleration of Numerical Linear Algebra

Numerical linear algebra has been widely applied in high performance computing to solve scientific and engineering problems. It requires computing systems to have huge computation capacity, and data throughput as problem size is increased. Although many methods have already been proposed to speed up computation through parallel programming in supercomputers or cluster systems, both memory wall and power wall problems prohibit system performance and power efficiency improvements resulting from technology scaling and instruction level parallelism. Therefore, how to reduce power consumption while increasing computation performance is one of the core concerns in current high performance computing (HPC) systems. On the other hand, hardware specialization in the form of GPUs, FPGAs, and ASICs offers a promising path toward major leaps in processing capability while achieving high energy efficiency. Particularly, with the development of semiconductor technology, FPGAs provide high energy efficiency, and have been widely applied in acceleration on computationally intensive applications, such as deep learning, data center. In this research, a low power and high performance FPGA-based accelerator for matrix-matrix multiplication is designed, and will finally extend the architecture to support other linear algebra algorithms.

Fig 3.5 shows the accelerator based on the systolic architecture, in which a processing element (PE) array was used to carry out the computation. In Fig. 3.5, the elements of matrices A and B are input into the computing engine horizontally and vertically from the block RAMs inside FPGA, and they are shifted rightward and downward cycle by cycle along computation, respectively. Each PE is a multiplier-accumulator and performs multiplications by one row and one column of matrices, and all PEs worked in parallel to perform multiplications of multiple rows and columns of matrices. Furthermore, a data reuse scheme and a novel memory hierarchy are proposed to speed up data access. The accelerator is developed through a combination of hardware/software co-design and algorithm/architecture co-design. The acceleration system with 16 × 16 PEs, and matrix multiplication up to the scale 20480 × 20480 in double precision will be finally verified and implemented by the FPGA board VC 709 from Xilinx, DE5 NET from Altera, and Intel's HARP system. Their performance will be evaluated through comparisons with other solutions, such as many-core PC and GPU. Intel approved us to remote access to a centralized FPGA cluster based on its non-released product, which contained a 12-core Intel microprocessor and an Arria-10 FPGA in a multi-chip package.

3.3.6 Advanced Approaches for Numerical Analysis

3.3.6.1 MTDM (Meshless Time-Domain Method)

In the simulation by using the finite-difference time-domain method (FDTDM), since nodes of electric and magnetic fields have to be arranged based on an orthogonal grid, it is difficult to treat the complex shaped domain including a curved surface. It is expected that the meshless time-domain method (MTDM) which applied a meshless method to the FDTDM is effective for a simulation in the complex shaped domain. Because it is indispensable to cope a large-scale simulation, we developed the basis simulation code using the 3-D MTDM in FY2015. In FY2016, we worked on speed-up of the time-dependent part of the simulation code. Concretely, the identical calculation patterns are identified in part of the MTDM core, and we can unify them into one operation. However, since a computational cost to identify the part which performs the identical calculation is large, it did not lead to dramatic speedup. In order to realize speedup, reduction of the computational cost to identify the part which performs the same calculation is essential. Accordingly, we performed the oral presentation in NAS 2016 [30].

3.3.6.2 Parareal (Parallel in time integration)

Recently, the number of computational core increase drastically due to the improvement of many-core and parallel computation technology. It is expected that the number of computational cores becomes more than 100 million in the next-generation super computer. If recent technology is applied to the next-generation computer system, suitable calculation efficiency may not be performed. It is indispensable to develop the new parallel computing technology based on the next-generation computer system. In the present study, time is receiving the most attention as a new axis of parallelization. The article about time parallel computation was published since 50 years ago. However, it did not develop because computational accuracy was very low. The computational accuracy drastically improved by Parareal method published in 2001, the time parallel computation using Parareal method reaches the practical use level In FY2016, we investigated the basic theory of Parareal method and its application field, and presented at the auto-tuning micro workshop [31].

3.4 Schedule and Future Plan

3.4.1 KMATHLIB2 and novel Numerical Algorithms

For the studies of KMATHLIB, the first milestone, which we design and build a prototype of a generic programming framework for the scientific parallel program, was completed during FY2012-2016. Enhancing KMATHLIB, we have started a new project to develop KMATHLIB2, which is intended to be a future bridge between user API and numerical library for more flexible parallel processing, for example, concurrent of multiple thread teams. In FY2017-19, we review and investigate:

- task-based numerical libraries,
- parallel programming languages, and
- parallel runtime systems.

We are going to design KMATHLIB2 and prototype implementations. Then, we implement the whole system from FY2019 to FY2022.

For the study of each numerical algorithm, we continue to develop an implementation of eigensolver and series of communication avoiding algorithms such as CACG, CAGMRES, CAQR, 2.5D algorithms, multi-axis decomposition FFT, and so on. Also, new numerical principle to compute eigenvalue, such as the spectral divide and conquer method base on the polar-decomposition, is our challenging work to the next step of the EigenExa library.

From FY2017, we receive a new fund, which supports the research for Tensor Network (TN) scheme, and have started a new project to develop a batched SVD solver, and a high performance numerical tensor library, which contains a parallel Decker decomposition and a parallel CP decomposition.

$$\mathcal{A} = \sum_{r=1}^{R} \mu_r u_r^{(1)} \circ u_r^{(2)} \circ \cdots \circ u_r^{(N)}$$

The tensor decomposition has higher complexity of flops and parallelism, and consequently it would apply to usage of accelerators as well as FPGAs described in the next subsection.

3.4.2 Future Devices for Numerical Computation (GPU, Manycore and FPGA)

Recent GPU technologies are truly focused on deep-learning, and half-precision accumulator and tensor calculator are installed on a next generation NVIDIA GPU, so called Volta processor. As we already studied Intel Xeon Phi, Knight Corner, processor, new generation Knight Landing must be evaluated for numerical linear algebra and other numerical libraries. Also, another high performance accelerator of PEZY-SC2 will be coming within FY2017. Therefore, broad-range of new architecture must be investigated systematically. It might be a good theme to build a new benchmark package for GPU and MIC concerning a numerical algebra such as multi-precision BLAS kernels, multi-dimensional FFT, eigensolver, tensor decomposition, and random number generator.

For the FPGA study, the designed accelerator device will be debugged, evaluated, and extended to other linear algebra algorithms. The design tradeoffs between power and performance will be investigated and analytical models for architectural tradeoffs will be researched to provide a deep insight on energy efficient linear algebra accelerators and explore limitations in current and future architectures for energy efficiency. The performance tuning of an FPGA-based acceleration system will be discussed, and potentials of using FPGA in HPC will be examined.

3.4.3 Advanced Numerical Analysis (Parareal)

For the Parareal study, we pursue to develop a preliminary code in order to examine feasibility of the Parareal method to several types of partial differential equation. Also, we evaluate characteristics of the parallel performance on various supercomputer systems in order to promote the Parareal method in practical simulation fields, such as fluid dynamics, particle simulation, and so on.

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Chapter 4

HPC Usability Research Team

4.1 Members

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Yumeno Kusuhara (Assistant)

4.2 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: computing portal systems, virtualization, and program analysis/verification.

4.2.1 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.

4.2.2 Virtualization

Virtualization is a technology for realizing virtual computers on real (physical) computers. One big problem of the abovementioned 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.

4.2.3 Program Analysis/Verification

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

4.3 Research Results and Achievements (FY2012 $\sim$ FY2016)

In this section, we summarize all the research results and achievements from FY2012 to FY2016 because the current research activities of the HPC Usability Research Team have come to an end in FY2016 and the new activities start from FY2017.

4.3.1 Design and Implementation of a Computing Portal Framework for HPC

As a first step of designing and implementing a computing portal framework that can be used by wide range of users, in FY2012, 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.

In FY2013, based on the prototype design and implementation of a computing portal framework of FY2012, we actually developed a prototype user-interface for the computing portal framework. More specifically, we implemented a web interface that runs on users web browsers and directly communicates with the backend system of the computing portal under the protocol (also designed in FY2012). With the web interface, software developers can easily publish their applications installed in HPC systems. For example, developers can specify the paths to the executables of their applications, parameters of their applications, and so on, via the web interface. In addition, developers can manage user accounts that are allowed to execute their applications. With the same web interface, users are also able to launch jobs. For example, users can select an application published in the computing portal, make an application to developers for using it, launch jobs by executing the application with arbitrary parameters, and manage the launched/exited jobs.

One feature of the implementation is that the communication protocol between the framework and its clients is based on the popular web-based application frameworks (e.g., WebSockets, JSON, etc.). Therefore, developers can develop their own custom interfaces for their applications if the web interface of our framework does not satisfy their requirements. Another distinguishing feature of our framework is that users can use portable

devices (e.g., smartphones, mobile tablets, and so on) because our web interface is carefully designed so that it can be viewed and accessed with any screen size.

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

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

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

In FY2015, we further enhanced the computing portal framework so that the users of the K computer are able to build and publish their own computing portal with their own authority and computing resources on the K computer.

In FY 2016, we further improved the implementation. Especially, we improved its compatibility and interoperability with computing systems other than the K computer, and designed/implemented a point system that is able to manage computing resources among users. In addition, we demonstrated the implementation at the open house of AICS.

4.3.2 Virtualization Techniques

4.3.2.1 Lightweight Virtualization for Testing/Debugging Parallel Programs

In order to utilize the full power of todays 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 abovementioned 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.

In FY2013, we have implemented a prototype of our lightweight virtualization system based on the design of FY2012. Although there still remained bugs, it successfully ran on conventional PC clusters and Fujitsus FX10. More specifically, several MPI applications (including some of the NAS parallel benchmarks (NPB)) ran on our prototype virtualization system. In addition, we also ran Scalasca (a network performance profiling tool) on our system.

In FY2014 and FY2015, we improved the prototype of our lightweight virtualization system and it successfully ran on the K computer. More specifically, it successfully ran 20000 virtual computing nodes on 1000 physical computing nodes. Because the operating system kernel of the computing nodes of the K computer has a serious fault which is related to memory management, we could not increase the number of virtual computing nodes at that time.

In FY2016, we further improved the implementation in order to work around the abovementioned bug, and it successfully ran on 40000 virtual computing nodes on 2000 physical computing nodes of the K computer. In theory, it must be able to run more virtual computing nodes on a single physical computing node and run on more physical computing nodes, but this is not possible so far because the K computer restricts the number of user processes on a physical computing node.

4.3.2.2 Container Technologies for HPC

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

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

The reason why the conventional HPC systems are less flexible and/or responsive is that their primary purpose is to compute scientific applications efficiently as much as possible, thus the overheads that may be introduced by utilizing full virtualization technologies are unacceptable.

On the other hand, as described above, the recent advance in the container technologies achieves very small overheads yet provides sufficiently flexible virtual execution environments, thus we predict that the container technologies will play important role in forthcoming HPC usage.

Based on the abovementioned perspective, we are studying the possibilities of applying the container technologies (especially, Docker) to the HPC systems. More specifically, in FY2013 and FY2014, we developed dockerIaaSTools (`https://github.com/pyotr777/dockerIaaSTools`), which enables us to easily setup isolated multiple virtual execution environments to which users are able to login via SSH. In addition, as an application

of dockerIaaSTools, we extended K-scope (`http://www.aics.riken.jp/ungi/soft/kscope/`), which is a Fortran source code analysis tool developed by Software Development team of AICS, so that users are able to use the backend of K-scope that is installed in the remote server seamlessly as if it is installed in their local computers. Moreover, we also studied the internals of Docker and developed extensions that enable us to conserve storage for storing images containers (e.g., `https://github.com/pyotr777/docker-registry-driver-git`). Furthermore, as described above, we integrated Docker with our computing portal framework.

In FY2015, we also utilized Docker to improve the usability of K-scope. More specifically, we created a Docker container image in which K-scope is installed so that users are able to use K-scope without manually installing it. In addition, we also extended K-scope so that users are able to analyze their programs seamlessly on the remote server without modifying their source code and/or build scripts.

4.3.3 Program Verification and Analysis

4.3.3.1 Software Model Checking for Partitioned Global Address Space Language

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 that is essential to achieve high performance on massively-parallel distributed memory systems of today (and future).

Despite the abovementioned 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.

4.3.3.2 Memory Consistency Model-Aware Program Verification

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

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

To address the problem, in FY2013, we studied three approaches. First approach is to define a new formal system that is able to represent various relaxed memory consistency models. More specifically, we define a very relaxed memory consistency model as a base model. On top of the base model, we defined various memory consistency models as additional axioms. With our formal system, we are able to define a broad range of memory consistency models from CPUs to shared-memory programming languages (e.g, Intel64, Itanium, UPC, Coarray Fortran, and so on), in the single formal system. With our formal system, we were able to proof the correctness of Dekkers mutual exclusion algorithm under the memory consistency model of Itanium.

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

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

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

In FY2015, we further improved the implementation of McSPIN and studied the memory consistency model

of the programing language Chapel by request from a research developer of Chapel. Moreover, we also studied several memory management algorithms on various memory consistency models with external researchers.

In FY2016, we studied a unified and versatile theory for program analysis/verification under various relaxed memory consistency models, and enhanced/improved the implementation of McSPIN further. Especially, we used McSPIN for analyzing/verifying various concurrent copying garbage collection algorithms and various relaxed memory consistency models.

4.3.3.3 Evidence-Based Performance Tuning

In order to fully utilize the power of HPC systems, it is necessary to optimize and tune the performance of applications. However, performance tuning is a troublesome task because, even if performance bottlenecks/hotspots can be detected by performance profiling, it is not apparent how to rewrite programs to remove the bottlenecks/hotspots. In addition, generally speaking, modifying correctly working programs is reluctant from the viewpoint of developers. Thus, performance tuning requires experienced craftsmanship, and relies on intuition and experience.

In order to address the problem, we are working on an idea of evidence-based performance tuning. More specifically, we store the results of performance profiling in a database where the results are associated with source code modification history. With the database, developers are able to know, for example, what kinds of optimization were applied in the past, what kinds of optimization are effective for improving a certain performance profiling parameter, and so on. In FY2013, we conducted a preliminary experiment to implement the database and obtained promising results.

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

In FY2015, we tried to increase the number of tuning cases in order to conduct detailed evaluation and improve accuracy of the analysis, but it turned out that it is hard to collect data directly because we could not find any researcher/developers who have such the data in and out of AICS. To work around the problem, we studied an approach of predicting performance of programs only from their source code modification history.

In FY2016, we further pursued the abovementioned approach of FY2015. More specifically, we designed and implemented an approach which is able to associate source code modification history with estimated performance data obtained by utilizing a B/F prediction approach without performing actual performance profiling. In fact, we analyzed several thousands of Fortran projects registered in GitHub (`https://github.com`), and were able to know their estimated performance characteristics.

4.3.3.4 Python-Based Aggregation of Multiple Software for HPC

In the world of HPC, programs are usually written in somewhat old-fashioned programing languages such as Fortran/C/C++ for historical reasons, thus writing programs for HPC is painful because we cannot use useful features of modern sophisticated programming languages. On the other hand, it is not realistic so far to write a whole program in modern programing languages because of performance problems.

In order to address the problem and achieve both productivity of program development and performance of program execution, we studied an approach of using Python for writing HPC applications. More specifically, we write non-performance critical large part of a program in Python, and performance critical small part in Fortran/C/C++. The reason why we choose Python is that Python provides a rich set of foreign language interfaces. For example, Fortran programs can be interfaced with f2py (NumPy: `http://www.numpy.org/`), C

programs can be interfaced with ctypes and Cython, and C++ programs can be interfaced with Boost.Python and Cython.

In FY2013, we modified EigenExa (a high-performance Eigen-solver developed by the Large-scale Parallel Numerical Computing Technology research team of AICS) so that it can be used as a shared library and a Python module (these modifications were feedbacked to the upstream). In addition, integration of Lotus (a quantum chemistry library developed by Dr. Tomomi Shimazaki, the Computational Molecular Science research team of AICS) and EigenExa were ongoing mainly by Tomomi Shimazaki.

In FY2014, in collaboration with Dr. Tomomi Shimazaki, a non-performance critical large part of Lotus was refactored and written in Python. We were able to utilize various existing libraries (e.g., EigenExa: `http://www.aics.riken.jp/labs/lpnctrt/EigenExa_e.html`, SMASH: `http://smash-qc.sourceforge.net/`, ASE: `https://wiki.fysik.dtu.dk/ase/`, etc.) in Lotus with the refactoring, and demonstrated that the features of Lotus can be easily extended. More specifically, we extended Lotus by request of Yukio Kawashima of the Computational Chemistry research unit of AICS with only several tens of lines of code addition.

In FY2015 and FY2016, we further refactored Lotus by using Cython, and our Python approach has been practiced by Dr. Kazuo Kitaura for realizing his new quantum chemistry calculation theory, with the help of Dr. Tomomi Shimazaki. In addition, we examined an approach of constructing a database that stores the results of ab initio calculations for molecules of PubChem (a famous chemical database of molecules), and applying machine learning and data mining approaches on the database. More specifically, we conducted several preliminary experiments utilizing machine learning approaches and performance evaluation of elemental technologies for constructing the database.

4.3.3.5 Porting Performance Analysis Tools to the K computer

Because massively parallel supercomputers, such as the K computer, are very different from single computer systems or small size cluster systems, simply porting existing applications to the K computer typically does not work due to performance problems (many existing conventional applications do not consider massively-parallel systems). Therefore, performance profiling is necessary to understand the behaviors of applications on massively parallel systems and tune the applications.

To address the problem, we are porting/deploying existing performance analysis tools to the K computer, in cooperation with external research institutes. More specifically, in FY2014, we ported two performance analysis tools to the K computer: Scalasca (`http://www.scalasca.org/`) and Extrae (`https://www.bsc.es/computer-sciences/extrae`). Scalasca was ported in cooperation with a research team of Juelich Supercomputing Centre, and Extrae was ported in cooperation with a research team of Barcelona Supercomputing Center. Using the ported tools, we actually analyzed the behavior of ABySS (`http://www.bcgsc.ca/platform/bioinfo/software/abyss`), a parallel genome sequence assembler. We also analyzed the behavior of SIONlib, a parallel I/O library, in cooperation with J 端 lich Supercomputing Centre, and deployed it on the K computer.

In FY2015, we continued to port/deploy existing performance analysis tools to the K computer. Especially, we ported Eclipse PTP (`https://eclipse.org/ptp/`), which is an extension framework of Eclipse (`https://eclipse.org/`) for parallel program development/execution, to the K computer, in cooperation with a research team of University of Oregon. In addition, we modified and integrated Extrae and SIONlib so that Extrae is able to use SIONlib for its I/O processing (this should be useful for handling very large trace data).

In FY2016, we further improved the ported implementation of Extrae for the K computer in cooperation with a research tea of Barcelona Supercomputing Center, and published it on the K computer. In addition, we conducted performance analysis of several applications on the K computer. For example, we analyzed the performance of the brain simulator NEST, and published the results of the analysis as a reviewed journal article. We also ported and analyzed libraries for machine learning (deep-learning, especially) on the K computer.

4.4 Schedule and Future Plan (FY2017 ∼)

From FY2017, the HPC Usability Research Team aims to increase the number of applications of the K computer. It especially focuses on applications that make use of both simulation and data analysis. We expect that the combination of simulation and data analysis will increase the value of both components because data can improve simulation accuracy and simulations can generate valuable data. However, developing such combined applications is difficult because developers must have expertise in computer systems, as well as simulation and data analysis algorithms, to connect the different types of programs. Our team studies tools and frameworks

that simplify the process of developing and executing such combined applications so that more people, especially those in industry, can use the supercomputer for their innovative products and services.

More specifically, we will study software for creating data analysis workflow and framework for combining data analysis and numerical calculation.

4.5 Publications (FY2012 ∼ FY2016)

4.5.1 Journal Articles

[1] Abe, T. and Maeda, T.: "Concurrent Program Logic for Relaxed Memory Consistency Models with Dependencies across Loop Iterations", Journal of Information Processing 25:244-255. Jan. 2017.
https://doi.org/10.2197/ipsjjip.25.244

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https://doi.org/10.1007/978-3-319-50862-7_4

[3] Abe, T. and Maeda, T.: "A General Model Checking Framework for Various Memory Consistency Models", International Journal on Software Tools for Technology Transfer (2016). Jul. 2016.
https://doi.org/10.1007/s10009-016-0429-y

4.5.2 Conference Papers

[4] Hashimoto, M., Terai, M., Maeda, T, and Minami, K.: "An Empirical Study of Computation-Intensive Loops for Identifying and Classifying Loop Kernels", In Proceedings of the 8th International Conference on Performance Engineering (ICPE 2017), pp. 361-372, Apr. 2017.
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https://doi.org/10.1007/978-3-319-47958-3_4

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[9] Abe, T. and Maeda, T.: "Towards a Unified Verification Theory for Various Memory Consistency Models", In Proceedings of the 6th Workshop on Syntax and Semantics of Low-Level Languages (LOLA 2015), Short Paper, online, Kyoto, Japan, Jul. 5, 2015.

[10] Hashimoto, M., Terai, M., Maeda, T., and Minami, K.: "Extracting Facts from Performance Tuning History of Scientific Applications for Predicting Effective Optimization Patterns", In Proceedings of the 12th Working Conference on Mining Software Repositories (MSR 2015), pp. 13-23, Florence, Italy, May 16, 2015.
https://doi.org/10.1109/MSR.2015.9

[11] Abe, T. and Maeda, T.: "Optimization of a General Model Checking Framework for Various Memory Consistency Models", In Proceedings of the 8th International Conference on Partitioned Global Address Space Programming Models (PGAS 2014), pp. 14:1-14:10, Eugene, OR, USA, Oct. 10, 2014.
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[12] Terai, M., Bryzgalov, P., Maeda, T., and Minami, K.: "Extending K-scope Fortran Source Code Analyzer with Visualization of Performance Profiling Data and Remote Parsing of Source Code", In Proceedings of the 6th International Symposium on Advances of High Performance Computing and Networking (AHPCN) within International Conference on High Performance Computing and Communications (HPCC-2014), pp. 878-885, Paris, France, Aug. 22, 2014.
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[15] Abe, T., Maeda, T., and Sato, M.: "Model Checking Stencil Computations Written in a Partitioned Global Address Space Language", In Proceedings of the 18th International Workshop on High-Level Parallel Programming Models and Supportive Environments (HIPS 2013). pp. 365-374, Cambridge, MA, USA, May 20, 2013.
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4.5.3 Posters and Presentations

4.5.3.1 Posters

[17] Abe, T. and Maeda, T: "Research on Program Verification Considering Various Memory Consistency Models", The 13rd Dependable System Workshop (DSW2015). Poster. 2015. In Japanese.

[18] RIKEN AICS HPC Usability Research Team: "HPC Usabiilty Research Team", Exhibition of International Supercomputing Conference (ISC) High Performance. Poster. 2015.

[19] Bryzgalov, P.: "Eclipse PTP and TAU with K and FX10 Supercomputers", Exhibition of International Supercomputing Conference (ISC) High Performance. Flyer. 2015.

4.5.3.2 Invited Talks

[20] Maeda, T.: "Trial Study on Development of a Quantum Chemistry Library with Modern Programming Techniques", The 1st Workshop on High Performance Computing Chemistry (HPCC 2015), Kobe, Japan, Dec. 1, 2015. In Japanese.

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

4.5.3.3 Presentations

[22] Kitayama, I.: "DynInst on arm64 – Status", Linaro Connect Budapest 2017.

[23] Abe, T.: "Compositional Concurrent Program Logic for Relaxed Memory Consistency Models", Workshop on Computer Science and Category Theory (CSCAT 2015). 2015. In Japanese.

[24] Kitayama, I.: "Parallel File I/O Optimization with SIONlib", Japan Lustre Users Group 2014 (JLUG 2014). 2014.

[25] Hashimoto, M.: "Constructing Finge-Grained Tuning Cases Database and Its Application for Prediction of Effective Program Optimizations", The 10th Autotuning Research Group's Open Academic Session (ATOS10). 2014. In Japanese.

[26] Abe, T.: "Towards Semi-automatic Theorem Proving Considering Memory Consistency Models", The 25th Algebra, Logic, Geometry and Informatics (ALGI). 2014. In Japanese.

[27] Abe, T.: "Program Verification for Formalized Relaxed Memory Consistency Models", The 31st Symbolic Logic and Computer Science (SLACS). 2014. In Japanese.

[28] Kitayama, I.: "A User's Experience with FEFS", In Japan Lustre User Group 2013. 2013.

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

4.5.4 Patents and Deliverables

4.5.4.1 Patents

[30] "Program analysis/verification service provision system, control method for same, computer readable non-transitory storage medium, program analysis/verification device, program analysis/verification tool management device", Assignee: Japan Science and Technology Agency, Inventor: Toshiyuki Maeda, US Patent No.9400887, Japan Patent No.5540160, and so forth.

4.5.4.2 Deliverables

[31] CCA/EBT: Code Comprehension Assistance for Evidence-Based performance Tuning, `https://github.com/ebt-hpc/cca`, 2017∼

[32] Eclipse PTP ported for the K computer, `https://github.com/pyotr777/EclipsePTP_PJM_TSC/`, 2015∼

[33] McSPIN. `https://bitbucket.org/abet/mcspin`, 2014∼

[34] Python ported to the K computer. Available on the K computer. Simply do ". /opt/aics/hpcu/env.sh" on the computing nodes of the K computer, then follow the documents of Python, 2014∼

[35] NumPy ported to the K computer. Available on the K computer. Simply do ". /opt/aics/hpcu/env.sh" on the computing nodes of the K computer, then follow the documents of NumPy, 2014∼

[36] MPI4Py library ported to the K computer. Available on the K computer. Simply do ". /opt/aics/hpcu/env.sh" on the computing nodes of the K computer, then follow the documents of MPI4Py, 2014∼

[37] MapReduce-MPI library ported to the K computer. Available on the K computer. Simply do ". /opt/aics/hpcu/env.sh" on the computing nodes of the K computer, then follow the documents of MapReduce-MPI, 2014∼

[38] Python binding of Rokko (Integrated Interface for Libraries of Eigenvalue Decomposition) (joint work with Dr. Sakashita and Prof. Todo of the University of Tokyo. Feedbacked to the original source tree of Rokko), 2014∼

[39] TAU ported to the K computer. Available on the K computer, 2013∼

[40] Extrae ported to the K computer. Available on the K computer, 2013∼

[41] Scalasca ported to the K computer. Available on the K computer (Joint work with Programming Environment Research Team of AICS), 2013∼

[42] Python binding of EigenExa (joint work with Dr. Shimazaki of Computational Molecular Science Research Team of AICS. Partially feedbacked to the original source tree of EigenExa, developed by Large-scale Parallel Numerical Computing Technology Research Team), 2013∼

[43] DockerIaaStool: Tools for creating a simple Infrastructure-as-a-Service system with Docker, 2013∼

[44] K-scope with SSHConnect (joint work with Software Development team of AICS), 2013∼

Chapter 5

Field Theory Research Team

5.1 Members

Yoshinobu Kuramashi (Team Leader)

Yoshifumi Nakamura (Research Scientist)

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

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Takeshi Yamazaki (Visiting Scientist, University of Tsukuba)

Shinji Takeda (Visiting Scientist, Kanazawa University)

5.2 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

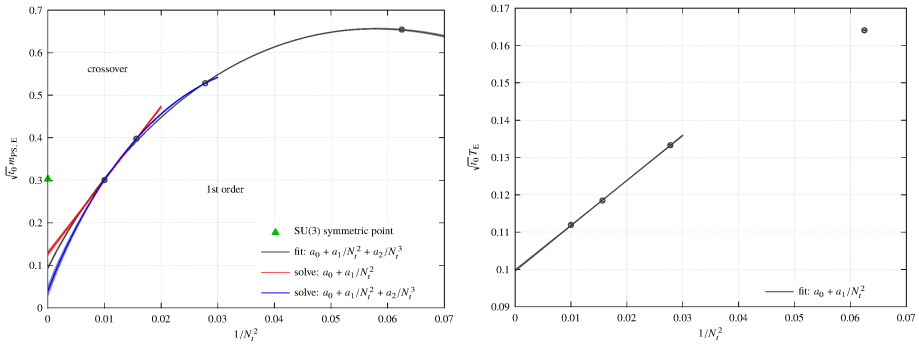


Figure 5.1: Continuum extrapolation of the critical point $\sqrt{t_0}m_{\rm PS,E}$ (left) and $\sqrt{t_0}T_{\rm E}$ (right) with $\sqrt{t_0}$ the Wilson flow scale.

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.

5.3 Research Results and Achievements

5.3.1 QCD at finite temperature and finite density

Establishing the QCD phase diagram spanned by the temperature T and the quark chemical potential μ in a quantitative way is an important task of lattice QCD. We have been working on tracing the critical end line in the parameter space of temperature, chemical potential and quark masses in 3 and 2+1 flavor QCD using the $O(a)$-improved Wilson quark action and the Iwasaki gauge action. We have determined the critical end point at zero chemical potential $\mu = 0$ in 3 flavor case. Our strategy is to identify at which temperature the Kurtosis of physical observable measured at the transition point on several different spatial volumes intersects. This method is based on the property of opposite spatial volume dependences of the Kurtosis at the transition point between the first order phase transition side and the crossover one. We have carried out a systematic study of the critical end point changing the temporal lattice size from $N_t = 4$ to 10, which corresponds to change the lattice spacing. In Fig. 5.1 (left and right panels) we show the continuum extrapolation of the critical pseudoscalar meson mass $m_{\rm PS,E}$ and the critical temperature $T_{\rm E}$ normalized by $\sqrt{t_0}$, where $\sqrt{t_0}$ denotes the Wilson flow scale. The latter shows a stable continuum extrapolation and we obtain $\sqrt{t_0}T_{\rm E}$=0.09932(39). The critical temperature in physical units is given by $T_{\rm E}$=134(3) MeV using the Wilson flow scale $\sqrt{t_0}$=1.347(30) GeV. On the other hand, $\sqrt{t_0}m_{\rm PS,E}$ shows significantly large scaling violation. In the extrapolation procedure, we try several fitting forms including up to cubic correction term and examine the fitting range dependence. As a result, their dependence turns out to be large as shown in Fig. 5.1 (left). The value of the upper limit is taken from the maximum continuum value among all the fits we did. In physical units, this bound is $m_{\rm PS,E} \lesssim 170$ MeV. At present we plan to make a simulation of finer lattice spacing to investigate the possibility that $m_{\rm PS,E}$ may vanish.

5.3.2 Nucleon form factors

Nucleon form factors are good probes to investigate the internal structure of the nucleon which is a bound state of quarks. Study of their properties requires nonperturbative method and much effort has been devoted to calculate them with lattice QCD since 1980's. Unfortunately, the current situation is that we are still struggling for reproducing the well-established experimental results, e.g., the axial vector coupling and the electric charge radius. This means that we have not yet achieved proper treatment of a single hadron in lattice QCD calculation. We focus on two major systematic uncertainties in the current simulations: one is heavier quark masses than the physical values and the other is finite spatial volume effects. In order to get rid of them we have carried out a calculation of the nucleon form factors on an $(8.1\ {\rm fm})^4$ lattice at almost the physical point in 2+1 flavor QCD. Thanks to the large spatial volume we can get access to small momentum transfer region up to 152 MeV. Here we present some preliminary results for vector form factors for the nucleon. In Fig. 5.2 we plot the Dirac

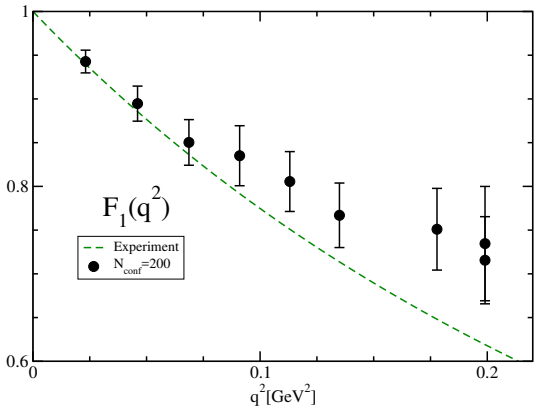


Figure 5.2: Dirac form factor as a function of the momentum transfer. Dotted green line denotes the experimental results.

form factor as a function of the momentum transfer. We observe a good consistency between our results (black circle) and the experimental values (dotted green line) especially at small q^2 region. This is important, because the electric charge radius is defined by the q^2 dependence of the form factor at vanishing q^2. We currently make careful analyses both for the vector and axial vector form factors.

5.3.3 Development of algorithms and computational techniques

5.3.3.1 Application of deflation method to lattice QCD

Eigenvalue problem for a given large sparse matrix is common across various computational sciences including lattice QCD. It is necessary to solve the Wilson-Dirac equation $Dx = b$ in lattice QCD, where D is an $N \times N$ complex sparse non-Hermitian matrix with $N = L_x \times L_y \times L_z \times L_t \times 3 \times 4$ the number of four dimensional space-time sites multiplied by the internal degree of freedom. In current typical simulations the dimension N is $O(10^9)$. In most cases of lattice QCD calculations our interest is restricted to $O(10^2 \sim 10^3)$ eigenvalues and corresponding eigenvectors around the origin. The removal of their subspace allows us to accelerate solving the Wilson-Dirac equation $Dx = b$. The following is an example of algorithm:

1. $P = 1 - \sum_k \phi_k \phi_k^\dagger$,
2. $PDx = Pb \Rightarrow DPx = Pb$,
3. $\psi = D^{-1} Pb$,
4. $\psi = Px = x - \sum_k \phi_k(\phi_k, x) = x - \sum_k \lambda_k^{-1}(\phi_k, b)$,
5. $x = D^{-1} Pb + \sum_k \lambda_k^{-1}(\phi_k, b)$

λ_k is the k-th smallest eigenvalue around the origin and the corresponding eigenvector is denoted by ϕ_k. P is a projection to remove the subspace corresponding small eigenvalues. This algorithm is useful to reduce the computational cost in solving $Dx^{(i)} = b^{(i)}$ with multiple right-hand side vectors $i = 1, \ldots, M$. Although the eigenvalues and corresponding eigenvectors are usually obtained by the Lanczos method, we have tried to apply the deflation method with Schwartz alternating procedure (SAP) proposed by Lüscher to a large scale Wilson-Dirac equation, where D is constructed with a state-of-the-art 2+1 flavor lattice QCD configuration on a 96^4 lattice at the physical point. We have found that the deflation technique successfully reduces the computational cost by a factor of 20 in solving the Wilson-Dirac equation with multiple right-hand side vectors. We currently work on improving the deflation algorithm and an optimization of the algorithmic parameters.

5.3.3.2 Tensor network scheme in path-integral formalism

The Monte Carlo simulation of lattice gauge theory is quite powerful to study nonperturbative phenomena of particle physics. However, when the action has an imaginary component like the θ term, it suffers from the

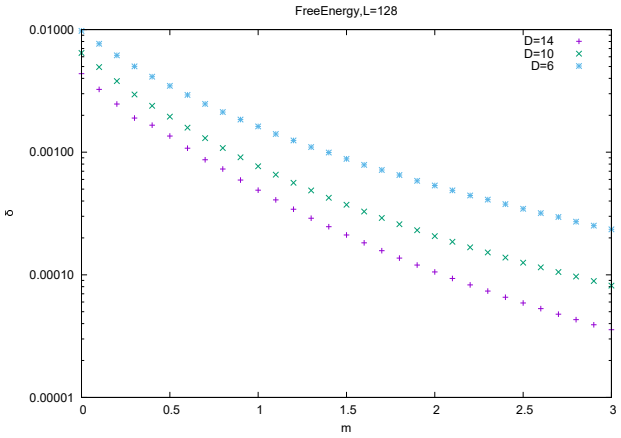


Figure 5.3: Deviation of the measured free energy with the GHOTRG algorithm from the exact one obtained by an analytic calculation on a 128^3 lattice as a function of the mass parameter m of the Wilson fermion. D denotes the parameter in the GHOTRG algorithm.

numerical sign problem, failure of importance sampling techniques. The effect of the θ term on non-Abelian gauge theory, especially quantum chromodynamics (QCD) is important, because it is related to a famous unsolved problem, "strong CP problem". The difficulty is also shared with finite density lattice QCD. So development of effective techniques to solve or by-pass the sign problem leads to a lot of progress in the study of the QCD phase diagram at finite temperature and density. The tensor network scheme is a promising theoretical and computational framework to overcome these difficulties. So far we have developed the Grassmann version of the tensor renormalization group (GTRG) algorithm in the tensor network scheme, which allows us to deal with the Grassmann variables directly. The GTRG algorithm was successfully applied to the analysis on the phase structure of one-flavor lattice Schwinger model (2D QED) with and without the θ term showing that the algorithm is free from the sign problem and the computational cost is comparable to the bosonic case thanks to the direct manipulation of the Grassmann variables. This was the first successful application of the tensor network scheme to a Euclidean lattice gauge theory including relativistic fermions. Toward the final target of 4D QCD we are currently working on three research subjects in the tensor network scheme: (i) non-Abelian gauge theories, (ii) higher dimensional (3D or 4D) models, and (iii) development of computational techniques for physical observables. In 2016 we have developed a Grassmann Higher Order Tensor Renormalization Group (GHOTRG), which is applicable to higher dimensional models. (GTRG is restricted to only two-dimensional models.) In order to check correctness and precision of the algorithm we have performed calculation of the free energy of 3D free Wilson fermion system. Figure 5.3 plots the deviation of the measured free energy with the GHOTRG algorithm from the exact one obtained by an analytic calculation on a 128^3 lattice as a function of the mass parameter m of the Wilson fermion. We present the results with $D = 6, 10, 14$, where D denotes the parameter in the GHOTRG algorithm. It is observed that the deviation diminishes as D is increased. We have successfully achieved a precision level of less than 1% for the region of $m \geq 0$, which assures the correctness of the algorithm and its ability for high precision calculation.

5.4 Schedule and Future Plan

5.4.1 QCD at finite temperature and finite density

We are now investigating the possibility that $m_{\mathrm{PS,E}}$ in 3 flavor QCD may vanish at the continuum limit making a simulation of finer lattice spacings. We have also started a systematic study of the critical end point in 4 flavor QCD.

5.4.2 Nucleon form factors

We are currently finalizing the analyses of the nucleon form factors calculated on an $(8.1\ \mathrm{fm})^4$ lattice at almost the physical point in 2+1 flavor QCD. After that we plan to perform a precision measurement of the form factors with larger lattice volume, which allows us to get access to smaller q^2 region.

5.4.3 Development of algorithms and computational techniques

5.4.3.1 Application of deflation method to lattice QCD

Our study reveals that the deflation method is quite efficient to reduce the computational cost in solving the large scale Wilson-Dirac equation with multiple right-hand side vectors. We plan to apply the deflation method to calculate various physical quantities in parallel with improving the algorithm.

5.4.3.2 Tensor network scheme in path-integral formalism

As stated above, there are three important subjects in research and development of tensor network scheme in path-integral formalism: (i) non-Abelian gauge theories, (ii) higher dimensional (3D or 4D) models, and (iii) development of computational techniques for physical observables. Future research follows these three directions.

5.5 Publications

5.5.1 Journal Articles

[1] Y. Kuramashi et al., "Critical endline of the finite temperature phase transition for 2+1 flavor QCD around the SU(3)-flavor symmetric point", Phys. Rev. D 94 (2016), p. 114507.

[2] QCDSF and UKQCD collaborations: R. Horsley et al., "QED effects in the pseudoscalar meson sector", JHEP04 (2016), p. 093.

[3] T. Muranushi et al., "Automatic generation of efficient codes from mathematical descriptions of stencil computation", FHPC2016 (2016), p. 17-22.

[4] T. Muranushi et al., "Simulations of Below-Ground Dynamics of Fungi:1.184 Pflops Attained by Automated Generationand Autotuning of Temporal Blocking Codes", Proceedings of the International Conference for High PerformanceComputing, Networking, Storage and Analysis, IEEE Press, 3 (2016).

[5] R. Horsley et al., "Isospin splittings of meson and baryon masses from three-flavor lattice QCD+QED", Journal of Physics G: Nuclear and Particle Physics, Volume 43 (2016).

[6] J. Dragos et al., "Nucleon matrix elements using the variational method in lattice QCD", Phys. Rev. D 94 (2016), p. 074505.

[7] Hiroya Suno et al., "Precise calculation of the triple-alpha reaction rates using the transmission-free complex absorbing potential method", Physical Review C94 (2016), p. 054607.

[8] Georg von Hippel, Thomas D. Rae, Eigo Shintani, Hartmut Wittig, "Nucleon matrix elements from lattice QCD with all-mode-averaging and a domain-decomposed solver: an exploratory study", Nucl. Phys. B914, 138-159 (2017).

[9] H. Kawauchi et al., "Tensor renormalization group analysis of CP(N-1) model", Physical Review D93 (2016), p. 114503.

[10] N. Nakamoto et al., "Computation of correlation functions by tensor renormalization group method", Sci. rep. of Kanazawa Univ. Vol. 60, p.11.

5.5.2 Conference Papers

[11] PACS Collaboration: K.-I. Ishikawa, Y. Kuramashi, N. Tsukamoto, S. Sasaki, T. Yamazaki, and A. Ukawa, "Nucleon form factors near the physical point in 2+1 flavor QCD", Proceeding of Science (LATTICE 2016) 158.

[12] PACS Collaboration: J. Kakazu, K.-I. Ishikawa, N. Ishizuka, Y. Kuramashi, Y. Nakamura, Y. Namekawa, Y. Taniguchi, N. Ukita, T. Yamazaki, and T. Yoshié, "Electromagnetic pion form factor near physical point in $N_f = 2 + 1$ lattice QCD", Proceeding of Science (LATTICE 2016) 160.

[13] PACS Collaboration: T. Yamazaki, K.-I. Ishikawa, Y. Kuramashi,and A. Ukawa, "Systematic study of operator dependence in nucleus calculation at large quark mass", Proceeding of Science (LATTICE 2016) 108.

[14] S. Takeda, X.-Y. Jin, Y. Kuramashi, N. Nakamura, and A. Ukawa, "Update on $N_f = 3$ finite temperature QCD phase structure with Wilson-Clover fermion action", Proceeding of Science (LATTICE 2016) 384.

[15] T. Boku, K.-I. Ishikawa, Y. Kuramashi, L. Meadows, M. D'Mello, M. Troute, and R. Vemuri, "A performance evaluation of CCS QCD Benchmark on the COMA (Intel® Xeon Phi™, KNC) system", Proceeding of Science (LATTICE 2016) 261.

[16] R. Horsley et al., "Partially conserved axial vector current and applications", Proceedings of Science (LATTICE 2016) (2017), p. 149.

[17] QCDSF/UKQCD Collaboration: J. Zanotti et al., "Transverse spin densities of octet baryons using Lattice QCD", Proceedings of Science (LATTICE 2016) (2017), p. 163.

[18] A. Chambers et al., "Hadron Structure from the Feynman-Hellmann Theorem", Proceedings of Science (LATTICE 2016) (2017), p. 168.

[19] R. Horsley et al., "Towards a determination of the ratio of the kaon to pion decay constants", Proceedings of Science (LATTICE 2016) (2017), p. 284.

[20] Renwick J. Hudspith, Randy Lewis, Kim Maltman, Eigo Shintani, "Strong coupling constant from Adler function in lattice QCD", Mod. Phys. Lett. A 31, 1630037 (2016).

[21] Hiroya Suno et al., "Three-alpha Radiative Reaction Processes At Low Temperatures", Proceedings of the 14th International Symposium on Nuclei in the Cosmos (2016).

[22] H. Suno et al., "Eigenspectrum calculation of the O(a)-improved Wilson-Dirac operator in lattice QCD using the Sakurai-Sugiura method", Proceedings of International Workshop on Eigenvalue Problems: Algorithms; Software and Applications, in Petascale Computing (EPASA), (2016).

[23] Eigo Shintani, "Progress of lattice calculation of light-by-light contribution to muon g-2", Nuclear and Particle Physics Proceedings, Volumes 273-275 (2016), 1624-1630.

[24] H. Kawauchi et al., "Phase structure analysis of CP(N-1) model using Tensor renormalization group", Proceedings of Science (LATTICE 2016) (2016), p.322.

[25] R. Sakai et al., "Tensor renormalization group approach to higher dimensional fermions", Proceedings of Science (LATTICE 2016) (2016), p.336.

5.5.3 Posters and Presentations

[26] Yoshinobu Kuramashi, "Tensor Network Scheme for Lattice Gauge Theories" (invited talk), Phase structure of lattice field theories − Japanese-German Seminars 2016 − (Niigata University, Niigata, Japan, September 26-28, 2016).

[27] Yoshinobu Kuramashi, "Nucleon form factors near the physical point in 2+1 flavor QCD" (talk), 34th International Symposium on Lattice Field Theory (Lattice 2016) (University of Southampton, Southampton, UK, July 24-30, 2016).

[28] Y. Nakamura, "Lattice QCD with CG and multi-shift CG on Xeon Phi" (talk), 5th JLESC workshop, ENS-Lyon, Lyon, France, June 27-29, 2016.

[29] Y. Nakamura, "Critical endline of the finite temperature phase transition for 2+1 flavor QCD around the SU(3)-flavor symmetric point" (talk), 34th International Symposium on Lattice Field Theory (Lattice 2016), University of Southampton, Southampton, UK, July 24-30, 2016.

[30] Y. Nakamura, "Critical endline of the finite temperature phase transition for 2+1 flavor QCD around the SU(3)-flavor symmetric point" (talk), XQCD 2016, Plymouth University, Plymouth, UK, August 1-3, 2016.

[31] Y. Nakamura, "Critical endline of the finite temperature phase transition for 2+1 flavor QCD" (talk), Autumn JSPS meeting 2016, , Miyazaki University, Japan, September 21-24, 2016.

[32] Y. Nakamura, "Critical endline of the finite temperature phase transition for2+1 flavor QCD around the SU(3)-flavor symmetric point" (talk), Japanese-German Seminar 2016, Niigata University, Niigata, Japan, September 26-28, 2016.

[33] Y. Nakamura, "Towards high performance Lattice QCD simulations on Exascale computers" (talk), 6th JLESC workshop, , RIKEN AICS, Kobe, Japan, November 30 - December 2, 2016.

[34] Hiroya Suno et al., "Three-alpha Radiative Reaction Processes At Low Temperatures" (poster), 14th International Symposium on Nuclei in the Cosmos. Niigata, Japan, June 19-24, 2016.

[35] Hiroya Suno, "Eigenspectrum calculation of large sparse non-Hermitian matrices in lattice QCD" (talk), 5th Joint Laboratory for Extreme-Scale Computing Workshop. Lyon, France, June 27-29, 2016.

[36] Hiroya Suno et al., "Precise calculation of the triple-alpha reaction rates using the transmission-free complex absorbing potential method" (talk), Workshop on Nuclear Cluster Physics 2016. Yokohama, Japan, November 14-17, 2016.

[37] Hiroya Suno, "Exploring eigensolvers for large sparse non-Hermitian matrices" (talk), 6th Joint Laboratory for Extreme-Scale Computing Workshop. Kobe, Japan, November 31-December 2, 2016.

[38] Hiroya Suno, "Algorithm and code development in lattice QCD using the K computer (talk). 6th Joint Laboratory for Extreme-Scale Computing Workshop. Kobe, Japan, November 31-December 2, 2016.

[39] E. Shintani, "EDM calculation on the lattice" (invited talk), ECT* workshop, Baryons over antibaryons: the nuclear physics of Sakharov, 25 July 2016, 29 July 2016, Torento, Italy.

[40] E. Shintani, "Lattice study of finite size effect in g-2 HVP" (talk), Towards high precision muon g-2/EDM measurement at J-PARC, J-PARC, Tokai, Japan, November 28-29, 2016.

[41] E. Shintani, "Lattice study of finite size effect in g-2 HVP" (poster), The international workshop on future potential of high intensity accelerators for particle and nuclear physics (HINT2016), J-PARC, Tokai, December 5-8, 2016.

[42] Takeshi Yamazaki, "Light nuclei and nucleon form factors from $N_f = 2 + 1$ lattice QCD" (invited talk), CCS-LBNL Collaborative Workshop 2016, University of Tsukuba, Ibaraki, Japan, May 12-13, 2016.

[43] Takeshi Yamazaki, "Direct calculation of light nucleus from lattice QCD" (invited talk), Phase structure of lattice field theories – Japanese-German Seminar 2016 –, Tokimate, Niigata, Japan, September 26-28, 2016.

[44] Takeshi Yamazaki, "Direct calculation of nucleus from lattice QCD" (invited talk), 8th symposium for discovery, unification, and creation of new knowledge from interdisciplinary computational science, University of Tsukuba, Ibaraki, Japan, October 17-18, 2016.

[45] Takeshi Yamazaki, "Direct calculation of light nucleus from lattice QCD" (invited talk), First Tsukuba-CCS-RIKEN joint workshop on microscopic theories of nuclear structure and dynamics, University of Tsukuba, Ibaraki, Japan, December 14-16, 2016.

[46] Takeshi Yamazaki, "Systematic study of operator dependence in nucleus calculation at large quark mass" (talk), 34th International Symposium on Lattice Field Theory (Lattice 2016), University of Southampton, Southampton, UK, July 24-30, 2016.

[47] Takeshi Yamazaki, "Systematic study of direct calculation of light nucleus at large quark mass" (talk), 2016 Autumn Meeting of the Physical Society of Japan, Miyazaki University, Miyazaki, Japan, September 21-24, 2016.

[48] Takeshi Yamazaki, "Study of operator dependence of direct calculation of light nucleus at large quark mass" (talk), 2017 Annual Meeting of the Physical Society of Japan, Osaka University, Osaka, Japan, March 17-20, 2017.

[49] S. Takeda, "Tensor networks" (invited talk), 34th International Symposium on Lattice Field Theory (Lattice 2016), Southampton, UK, July 26, 2016

[50] S. Takeda, "Tensor Renormalization group" (invited talk), University of Tokyo, Tokyo, Japan, May 15,2016

[51] S. Takeda, "Algorithm of Tensor Renormalization group" (invited talk), University of Tsukuba, Tsukuba, Japan, August 9,2016

[52] S. Takeda, "Phase structure of Nf=3 QCD at finite temperature and density by Wilson-Clover fermions" (poster), 34th International Symposium on Lattice Field Theory (Lattice 2016), Southampton, UK, July 26, 2016.

Chapter 6

Discrete-Event Simulation Research Team

6.1 Members

Nobuyasu Ito (Team Leader)

Hajime Inaoka(Research Scientist)

Yohsuke Murase(Research Scientist)

Naoki Yoshioka (Research Scientist)

Shih-Chieh Wang (Postdosctoral Researcher)

Tomio Kamada (Guest Researcher)

Takeshi Uchitane (Guest Researcher)

6.2 Research Activities

Discrete-event simulations cover much wider fields than discretized simulations of continuous models. They comprise various kinds of models, for example, particles, agents, automata, games and so on, and their applications are from material and biomedical sciences to ecological and environmental problems. Social designs and controls have becoming the more interesting target since so-called the "big data sciences" became popular.

One characteristic feature of discrete-event simulations is their variety both in model parameters and behaviors. Different parameters of discrete models often result in qualitatively quite different behaviors. For example, two particles just pass through when they do not collide with each other, but they will be scattered to different orbits when they collide. A automaton reacts specifically when their inputs satisfy its activation condition. A system with such discrete elemets will behaves unpredictable way. This feature is much different from the case of "continuous" simulations which are often characterized by continuous change in behaviors when input parameters are slightly modified.

Another feature of discrete-event simulations is its network structure. Relations between elements are often characterized by graphs and the graphs have usually nonuniform. For example, in a system of hard particles, colliding particles are connected and noncolliding ones are not. The connection changed at every collision. Another example is human relations. Some are friendly connected, and some are competing. Such human relations are known to be characterized by a small-world structure.

These features are typically observed in simulations of social systems, for example, traffic, economy and social relationship. The Discrete-event simulation research team(DESRT) have been elucidating future applications of the K and future supercomputers to such social simulation.

6.2.1 Parameter-space explorer: OACIS and CARAVAN

The DESRT has been developing job management tools named OACIS and CARAVAN to challenge the huge-parameter space, the first feature. The name OACIS is an abbreviation of "Organizing Assistant for Comprehensive and Interactive Simulations"[28],

The OACIS have been released for public use as an AICS software, and the CARAVAN is now being tested with its prerelease version. Both of these two tools are used with user's simulation and analysis softwares. A user register one's simulation and analysis softwares togather with their input parameters and available host computers to these tools, then the tools control submitting and analyzing jobs.

Each simulation and each analysis for many parameters will be properly processed by computers if they are specified correctly, but error will easily be introduced by human side. In this sense, supercomputers are demanding not only greater programming skill but also more reliable operation and smarter decision of simulation parameters. The OACIS and CARAVAN are designed to solve this demand. A difference of the two tools is number of jobs and/or parameter sets. The OACIS is designed for jobs up to $10^6 \sim 10^7$ different parameters, and the CARAVAN to 10^9 and more.

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

Applications and users of the OACIS have been growing in and out of AICS. In this year 2016, six versions were released. These versions have been improved and numerous bugs were fixed. Major improvements are the followings:

- Wrapper script `xsub` which absorbs differences of job schedulers of various host computers were installed.
- Version numbers of simulators and their managements were installed.
- Read-only mode was installed, which help to share data in OACIS with others.
- API to Ruby and Python was installed so that Ruby and Python program could operate OACIS.

Start-up lectures on the OACIS usage were held not only in AICS but also in other organization like AIST and NIMS.

The CARAVAN is coded with a PGAS language X10 implemented to the K computer. It is now under development and it will be released in following years.

6.2.2 Factors in a traffic simulation of the Kobe city

A simulator of the car traffic in the Kobe city had been developed in the DESRT[1], using the SUMO simulator[2].

Following the year 2015, factors of the simulated traffic had been analyzed with multivariate analysis of traffic flow correlation between any two road sections in this year 2016[7]. The Kobe city is devided into six areas as shown in Fig. 6.1, and numbers of cars starting from one area and going to one area for each simulation corresponding to six hours of real time are assigned as shown in Tab. 6.1. Origin and destination(OD) of each trip are selected randomly in specified area, and one simulation is executed. Simulations are repeated with independently sampled OD sets, and factor analysis of multivariate statistical analysis is done for traffic flows of road segments. Figure 6.2 shows number of estimated significant factors is plotted versus number of random samples. The more samples provide the more factors and about 130 factors are obtained with 3,000 and more samples. These results imply that the major traffic of the Kobe city is composed of these factors, and they will be usefule for assessments, control and designs of the traffic. Anyway, they are from our traffic simulator, and comparison and verification with the real traffic will be the next challenge.

Furthermore, fundamental behavior of network traffic was also studied. It is a challenge to extend so-called the fundamental diagram, which is a density-flux relation of road segment, to road network [5].

[1] Yuta Asano, Nobuyasu Ito, Hajime Inaoka, Tetsuo Imai and Takeshi Uchinane, Proceedings of the International Conference on Social Modeling and Simulation, plus Econophysics Colloquium 2014(Springer Proceedings in Complexity, ISBN 978-3-319-20590-8), p. 255-264, Tra?c Simulation of Kobe-City.

[2] Daniel Krajzewicz, Jakob Erdmann, Michael Behrisch, and Laura Bieker. " Recent Development and Applications of SUMO - Simulation of Urban MObility ", International Journal On Advances in Systems and Measurements, 5 pp. 128-138, December 2012.

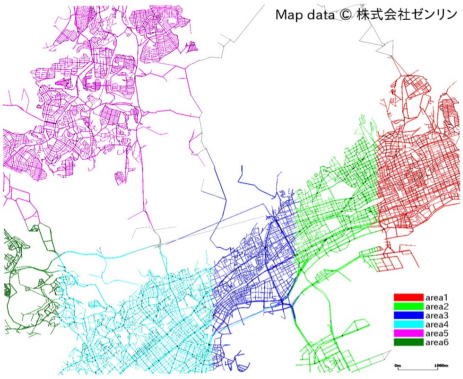


Figure 6.1: Areas 1 to 6 are shown with different colors.

		Departure					
		area1	area2	area3	area4	area5	area6
Arrive	area1	250	250	250	**8750**	250	250
	area2	250	250	250	250	250	250
	area3	250	250	250	250	250	250
	area4	**8750**	250	250	250	250	250
	area5	250	250	250	250	250	250
	area6	250	250	250	250	250	250

Table 6.1: Numbers of cars from area A in departure to area B in arrive are shown. Traffic between area 1 and 4 are 8750 trips in one way, which is larger than the other areas, 250, because of large traffic passing through the Kobe city.

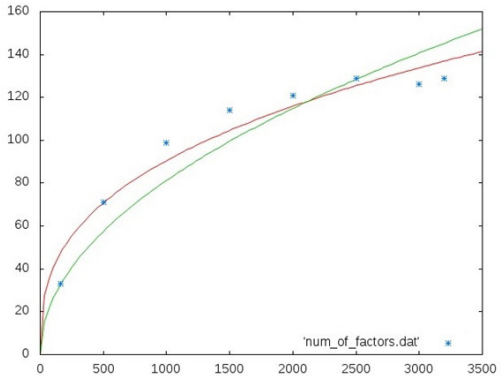


Figure 6.2: Number of estimated factors are plotted versus number of sampling numbers.

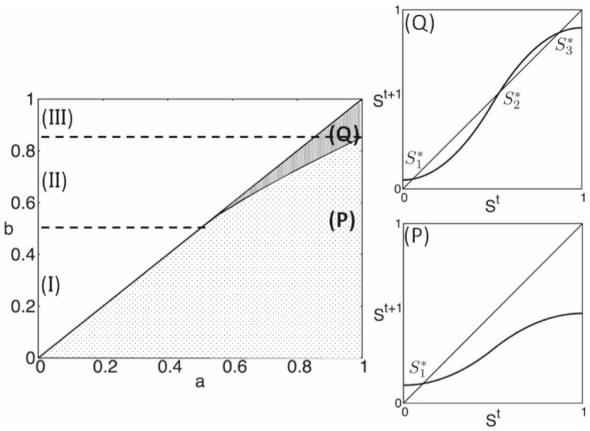


Figure 6.3: A typical regime diagram(left) of share distribution of two markets with share-sensitive traders is shown. It is for a case that a market B with tick size b is trying to get share from a giantic market A with tick size a. The relevant area $b \leq a$ is divided into two areas (P) and (Q). In area (P), only one equilibrium state exists, but in (Q) two stable equilibrium states exist. The market A succeeds to defend by keeping in the area (Q), and the market B will succeed to attack by keeping in the area (P)[6].

6.2.3 Competition strategy of stock exchange markets

When a trader sells or buys stocks, one orders to one of numerous stock exchange markets, and there are severe competition between markets. If a market is losing trade share, traders are not attracted to the market and go to another with big share. So markets are struggling to improve their trade rules to attract the more traders and to get the more share.

Control of tick size of stock price is known to be one of critical parameters of such market competition, which restricts call and put prices from traders. For example, when tick size of a stock is 10 yen, then traders can call or put at 990, 1000 and 1010 yen, but not at 995, 1005, 1015 yen. Smaller tick allows traders to order at a closer price for their expected price, but it makes chance of matching call and put orders. So an optimal tick size depends on atmosphere and environment of market and traders.

It had been studied with computer simulation using stylized trader agents how two markets with different tick sizes compete, and how a strategy for a small market to attach a giant market by adoping a smaller tick size works[3], In this year 2016, an analytic model which reproduces these results from simulations were proposed, and attack and defense strategies were proposed in cases with nonlinear preference of traders to share[6]. Fig. 6.3 shows one result in case of strong preference to share.

6.2.4 Evacuation planning

Well-prepared evacuation planning is critical to reduce and minimize damage of accident and disaster. Weak point and bottleneck of evacuation better be eliminated from the society, and evacuation simulations are useful to find them. Simulations can examine various disaster scenarios with various evaluation policies and plans, and visualization of results will clarify the situations.

In the year of 2016, various scenarios of evacuation plans in case of tsunami attack to Zaimokuza area of the Kamakura city were simulated with pedestrian agent model. Simulated area is shown in Fig. **??**. Simulation results of evacuation time that people in sea level areas B1 $\sim$ B7 escape to high areas F1 $\sim$ F3 are plotted for various population in Fig. 6.5. It is observed that population threshold which is about 4,000 exists. Above the threshold in case of local events or touristic season, evacuation process grows with population[8].

[3]T. Mizuta, S. Hayakawa, K. Izumi, and S. Yoshimura, JPX Working Paper Vol. 2 (2013).

Figure 6.4: Zaimokuza area in the Kamakura city is shown, together with starting low areas B1∼ B7 and safe high areas F1∼ F3.

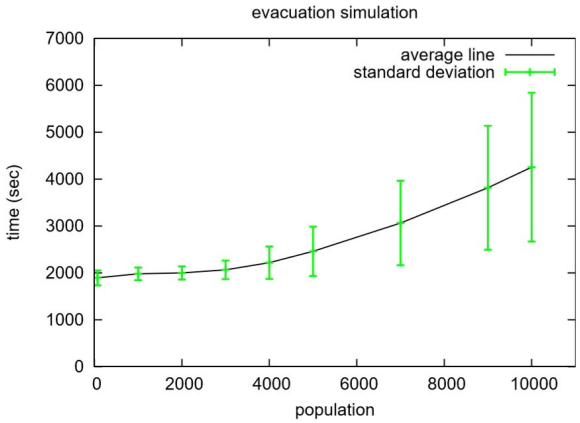


Figure 6.5: Simulation results of evacuation time for various population in the area are plotted. Up to about 4,000 people, evacuation time behaves flatly, and it increases for more people.

6.2.5 Other activities

In the year of 2016, following studies were published from this team:

1. Model development of human relationship[2,3]
2. simulation of granular materials[4]
3. Development of quantum gate computers
4. Molecular dynamics simulation of liquid-gas transition[1].

6.3 Schedule and Future Plan

From the research activities of DESRT so far, following problems are becoming clear:

1. Simulation models, typically social ones, comprise with large input parameters and output numbers, and their behaviors are strongly nonlinear with various regimes.
2. Social "big data" are often not big enough to picture details. It is clearly observed from our multivariate analysis of the traffic data[7]. Thousands of samples are necessary to get minor traffic factors, but such repetitions are not expected in the real traffic. Weather, economics, calendar, accidents and other factors varies every day.

For the first problems, application of so-called the "AI" will be challenged. For the second, controlled simulations will be one solution, and the way of the OACIS and the CARAVAN will realize them togather with development of simulation models for various phenomena.

6.4 Publications

6.4.1 Articles

[1]Hiroshi Watanabe, Hajime Inaoka, and Nobuyasu Ito, "Ripening kinetics of bubbles: A molecular dynamics study", Journal of Chemical Physics, vol. 145, 124707 (2016).
[2]Janos Torok, Yohsuke Murase, Hang-Hyun Jo, Janos Kertesz, Kimmo Kaski, "What does Big Data tell? Sampling the social network by communication channels", Physical Review E vol.94 (2016) 052319.
[3]Janos Kertesz, Janos Torok, Yohsuke Murase, Hang-Hyun Jo, Kimmo Kaski, "Multiplex Modeling of the Society", Manuscript for the Springer volume on Multiplex Network, within H2020 Multiplex Project.
[4]Akiyuki Kuwabara, Naoki Yoshioka, Takashi Shimada, and Nobuyasu Ito, "Drag force on two disks moving in a granular bed," Journal of Physics: Conference Series vol. 750 (2016) 012018.
[5]Naoki Yoshioka, Takashi Shimada, and Nobuyasu Ito, "Macroscopic fundamental diagram in simple model of urban traffic," Artificial Life and Robotics, (2016) DOI 10.1007/s10015-016-0345-y .
[6]Shota Nagumo, Takashi Shimada, Naoki Yoshioka, and Nobuyasu Ito, "The Effect of Tick Size on Trading Volume Share in Two Competing Stock Markets", Journal of the Physical Society of Japan vol.86 (2017) 014801.
[7]Takeshi Uchitane and Nobuyasu Ito, "Applying Factor Analysis to Describe Urban Scale Vehicfle Traffic Simulation Results," (in Japanese) Journal of the Society of Instrument and Control Engineers vol.52 (2016) No.10 p.545-554.
[8]Hiroyasu Matsushima, Takeshi Uchitane, Junpei Tsuji, Tomohisa Yamashita, Nobuyasu Ito and Itsuki Noda, "Applying Design of Experiment based Significant Parameter Search and Reducting Number of Experiment to Analysis of Evacuation Simulation," (in Japanese) Transactions of the Japanese Society for Artificial Intelligence vol.31 (2016) No.6 p.AG-E 1-9.

6.4.2 Invited Talks

[9]Y. Murase, "A software framework for comprehensive simulations and its application to social network modeling", Mini-workshop on Complex Systems and Networks, AIMR Tohoku University, Nov.24-25, 2016.
[10]Y. Murase, "Multilayer Weighted Social Network Model", Social Connectome, satellite meeting of NetSci2016, The K-Hotel, Seoul, Korea, May 30, 2016.

[11]Y. Murase, “Universality in Open-Evolving Systems”, The 4th International Workshop on Physics of Social Complexity, POSTECH, Korea, May. 27-28, 2016.
[12]N. Ito, ”Social simulations on the Post-K computer“, Asia-Pacific Econophysics Conference 2016 - Big Data Analysis and Modeling toward Super Smart Society - (August 24 - 26, 2016, Tokyo, Japan).
[13]N.Ito, ”Agent-based simulation of stock markets“, 2016 NCTS International Workshop on Critical Phenomena and Complex Systems (July 1-3, 2016, National Tsing Hua University, Shinchu, Taiwan)
[14]N.Ito, ”Agent-based simulation of stock markets“, 7th Hungary-Japan Bilateral Workshop on Statistical Physics of Breakdown Phenomena.

6.4.3 Oral Talks

[15] Y. Murase, “Sampling effects of communication channels on social networks”, Autumn Meeting of Physics Society of Japan(Kanazawa, Sep. 13-16, 2016)
[16] Y. Murase, “What does Big Data tell? Sampling the social network by communication channels”, The 1st Workshop on Self-Organization and Robustness of Evolving Many-Body Systems, Hotel Umehara, Ibaraki, Japan, August 27 and 28, 2016.
[17] Y. Murase, “Modeling the role of relationship fading and breakup in social network formation”, NetSci2016: International School and Conference on Network Science, The K-Hotel, Seoul, Korea, May 30-Jun 3, 2016.
[18] Naoki Yoshioka, “Burst size in fiber-bundle model revisited”, 2nd Funabashi Workshop on “Deformation and Fracture Dynamics”(Nihon University, Funabashi, Japan, Feb. 15-16, 2016).
[19] Naoki Yoshioka, Ferenc Kun, and Nobuyasu Ito, “Jump statistics of epicenters in thermally-activated fiber-bundle model”, 7th Hungary-Japan Bilateral Workshop on Statistical Physics of Breakdown Phenomena (Debrecen University, Debrecen, Hungary, May 4-5, 2016).
[20]Naoki Yoshioka, Takashi Shimada, and Nobuyasu Ito, “Macroscopic behavior and stability in urban traffic network”, The 3rd International Workshop on Physics of Social Complexity (Pohang University of Science and Technology, Pohang, Korea, May 27-28, 2016).
[21]Naoki Yoshioka, Hajime Inaoka, Nobuyasu Ito, Fengping Jin, Kristel Michielsen, and Hans De Raedt, “Simulations of quantum circuits on supercomputers”, International Workshop on Complex Phenomena from Molecule to Society (The University of Tokyo, Tokyo, Japan, Aug. 22-23, 2016).
[22]Naoki Yoshioka, Ferenc Kun, and Nobuyasu Ito, “Statistics of bursting events in fracture of fiber bundles”, The 1st Workshop on Self-Organization and Robustness of Evolving Many-Body Systems (Choshi, Japan, Aug. 27-28, 2016).
[23] Naoki Yoshioka, Ferenc Kun, and Nobuyasu Ito,” Jump statistics of epicenters in thermally-activated fiber-bundle model”, Hungary-Japan Workshop on Physics of Rheology and Fracture (Kyushu University, Hakata, Japan, Dec. 5, 2016).
[24]Naoki Yoshioka, Takashi Shimada, and Nobuyasu Ito, “Stability and macroscopic behavior in urban traffic network”, Nara Workshop on Nonlinear Dynamics (Nara Women’s University, Nara, Japan, Dec. 7-8, 2016).
[25]Nobuyasu Ito, ”Social simulations on HPC“, RIKEN AICS HPC Youth Workshop 2016(Nov.28-30, Kobe, Japan)
[26]Nobuyasu Ito, ”Social simulation with exascale computer“, (17th International Workshop on Computational Physics(CompPhys16, November, 24–26, 2016, Leipzig, Germany)
[27]Nobuyasu Ito, ”Social simulations on the Post-K computer” The 1st Workshop on Self-Organization and Robustness of Evolving Many-Body Systems (August 27–28, 2016, Ibaraki, Japan).

6.4.4 Software

[28] A job management application: OACIS, https://github.com/crest-cassia/oacis. Six releases of v2.5.0∼ v2.10.0 were made open in 2016, and it’s lectures were held at AICS, AIST, NIMS and so on.

Chapter 7

Computational Molecular Science Research Team

7.1 Members

Takahito Nakajima (Team Leader)

Tomomi Shimazaki (Senior Scientist)

Michio Katouda (Senior Scientist)

Noriyuki Minezawa (Senior Scientist)

Takehiro Yonehara (Senior Scientist)

Keisuke Sawada (Research Scientist)

William Dawson (Research Scientist)

Wataru Uemura (Research Scientist)

Robert van Meer (Research Scientist)

Rahul Maitra (Research Scientist)

Kizashi Yamaguchi (Visiting Scientist)

Kazuo Kitaura (Visiting Scientist)

Marek Wojcik (Visiting Scientist)

Muneaki Kamiya (Visiting Scientist)

Takashi Kawakami (Visiting Scientist)

7.2 Research Activities

7.2.1 Development of original molecular theory

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

a molecular theory and calculation methods to handle large complex molecules with high precision under a variety of conditions. To achieve our aim, we have so far developed several methods of calculation. Examples include a way for resolving a significant problem facing conventional methods of calculation, in which the calculation volume increases dramatically when dealing with larger molecules; a way for improving the precision of calculations in molecular simulations; and a way for high-precision calculation of the properties of molecules containing heavy atoms such as metal atoms.

7.2.2 New molecular science software NTChem

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

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

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

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

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

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

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

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

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

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

10). Efficient calculation for chemical reaction pathway.

11). Ab initio molecular dynamics calculation.

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

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

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

7.3 Research Results and Achievements

7.3.1 Large scale matrix polynomial computation for linear scaling quantum chemistry

In the self-consistent field loop of standard quantum chemistry codes, the density matrix is computed by using the eigendecomposition of the Hamiltonian matrix. This widely used approach has been able to take advantage

of massively parallel dense eigensolvers to compute the properties of systems with thousands of electrons using hundreds of thousands of CPU cores. However, the $O(N^3)$ complexity of solving the dense eigenvalue problem is a computational bottleneck that prevents diagonalization based quantum chemistry programs from treating significantly larger systems. To overcome this difficulty, a variety of reduced complexity, diagonalization free methods have been developed. At the core of these methods are the computation of matrix functions. With this in mind, we are currently developing a massively parallel library that can compute a variety of matrix functions. This library can not only be integrated into quantum chemistry programs, but also can be used for large scale calculations involving matrices from many different application areas. At the heart of this library are methods for computing matrix functions using polynomial expansions. One appealing feature of these polynomial expansions is that it allows one to compute matrix functions using just two core routines: matrix multiplication and matrix addition. In the case where the matrices involved are sparse, these routines can be replaced with sparse matrix multiplication and sparse matrix addition to allow computations that have costs that scale linearly with the size of the input systems. As a result, for all of the matrix functions implemented in our library, the bottleneck calculation is sparse matrix multiplication. With this in mind, we have invested considerable effort and computational time developing and tuning a massively parallel sparse matrix multiplication kernel. The parallelization of this routine was based on a communication avoiding matrix multiplication routine that had recently been proposed in the literature. We improved upon this routine by implementing a task based, MPI+OpenMP parallelization scheme to further improve parallel performance. With the core sparse matrix routines implemented, we then began building a number of matrix functions routines. For quantum chemistry calculations, we implemented a several different schemes for computing the density matrix, including different kinds of density matrix purification and methods based on minimization. We also implemented a range of generic matrix functions including trigonometric routines, the matrix exponential and logarithm, matrix roots, and general matrix polynomials. We have also implemented a number of supplementary routines that make it easy to integrate our library into a number of different codes. We recently evaluated our implementation of these methods using both synthetic data as well as real world data from many different quantum chemistry codes. Our results showed that our library demonstrates strong scale on up to 65,536 cores for even moderately sized problems. We have also made progress on the joint RIKEN and CEA project on Large Scale DFT calculations and QM/MM. First, we began by porting the BigDFT code to the K Computer. We wrote a configuration file that compiles BigDFT with the appropriate options on the K Computer. Several minor corrections to the source code and build system with made, after which BigDFT compiled successfully. We have utilized BigDFT on the K Computer to perform calculations on water molecule systems and to write representative matrices from these calculations to the file system. These matrices were then utilized for benchmarking our sparse matrix library.

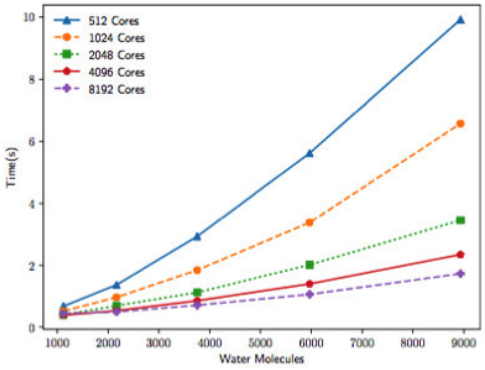


Figure 7.1: Time to compute the inverse square root of the overlap matrix of different sizes of water molecule clusters using the STO-3G basis set.

7.3.2 Development of distributed memory massively parallel code of the Hartree-Fock and second-order Møller-Plesset perturbation calculations for K computer

HF theory is a basic theory for the calculations of ground-state electronic structure of large molecules. Previously, we developed the MPI/OpenMP hybrid parallel code of HF calculations [T. Nakajima *et al.*, Int. J.

Quant. Chem. **115**, 349 (2015)] for the NTChem. The parallel scalability of this code is good up to about 10,000 MPI processes for molecules containing about 10,000 atomic orbitals (AOs) on the K computer. However, the calculations were limited for the size containing up to about 10,000 AOs due to a problem of memory demands which was derived from the replicated memory algorithm in the previous implementation. To overcome this problem, we have developed a new distributed memory MPI/OpenMP hybrid parallel code of HF calculations. In this code, we have applied a parallel algorithm of two-electron Fock matrix calculations where column blocks of Fock matrix and density matrix are statically distributed (Figure 7.2). We implemented this algorithm to NTChem using one-sided network communication application programming interface (API) in global array (GA) toolkit avoiding complicated two-sided network communication. The linear-algebra calculation in the HF self-consistent field calculations such as the matrix-matrix multiplication, diagonalization, and DIIS extrapolation of Fock matrix are parallelized using ScaLAPACK and EigenExa libraries. The new implementation is suitable for the HF calculations of very large molecules containing more than 10,000 AOs and 1,000 nodes on the peta-scale supercomputers such as the K computer.

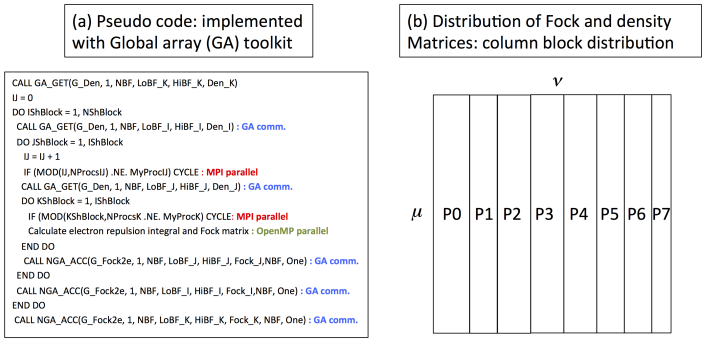


Figure 7.2: (a) pseudo code of distributed memory parallel Fock matrix calculation and (b) distribution of Fock matrix and density matrix.

7.3.3 Improvement of computational performance on pseudospectral method

A fast estimation of two-electron repulsive integrals (ERIs) is an important and imperative subject in any ab-initio quantum chemical calculations. Since the computational cost of the ERIs formally increases as N^4, where N is the number of basis functions, we often suffer from much time-consuming estimations in large molecular systems. In order to address the tough problem, several methodologies have been developed to date. Among them, the pseudospectral (PS) method is a strong candidate for a quick and efficient evaluation of the ERIs. In this method, one analytical integral is replaced by a numerical summation consisting of discrete grid points and the computational cost is reduced from $O(N^4)$ to $O(MN^2)$, where M is the number of grid points. Because of the discretization of a continuous integral space, the PS method is not only a fast method for estimations of the ERIs but also suitable for recent massively parallel computations using numerous CPU cores. In this fiscal year, we attempted to improve the performance of the PS method implemented in NTChem. In the PS method, it is necessary to calculate one-electron analytical integrals for whole real-space grid points. So far, one-electron analytical integrals were computed using subroutines of SMASH software. The SMASH subroutines are created to calculate one-electron term in Hamiltonian and not always optimal for current PS subroutines implemented in NTChem. On the other hand, because the SMASH subroutines have to be called from NTChem many times, the overheads for calling SMASH subroutines increase. To improve the computational efficiency and reduce the overheads, we independently developed subroutines that fit to the PS method in NTChem. In own developed subroutines, although the integral scheme adopts the same approach as SMASH, it is designed to reduce overheads as much as possible. In order to investigate the performance of own developed subroutines, we performed MPI/OpenMP hybrid parallel computations on the K Computer and compared the computational time for the estimation of ERIs between SMASH and own developed subroutines. Our calculations were based on a pure DFT and H_2O molecular cluster with 8,525 basis sets was employed as a test system. As shown in Table 7.1, by using own subroutines, we achieved a considerable reduction of the computational time.

The number of nodes	SMASH subroutines (s)	Own developed subroutines (s)
1024	92.76	43.10
2048	54.88	27.78
4096	34.92	20.65
8192	29.58	17.60

Table 7.1: Computational times for estimation of ERIs when using PS method

7.3.4 Development of the linear response two-component relativistic time-dependent density functional theory for molecular properties

We have recently developed the two-component relativistic TDDFT for excitation energies. In this method, as in the case of nonrelative calculations, a direct algorithm using a trial vector without integral transformations can be applied, so each excitation energy can be obtained with a similar computational cost of the ground-state energy. However, since this algorithm requires at least the same number of trial vectors as the number of excited states to be found, it is difficult to compute the excitation spectrum of the system of interest with this algorithm because of computer cost and storage limitation. In particular, the two-component relativistic time-dependent density functional theory treats the spin-flip excitation configuration in addition to the excitation configuration dealt with in the non-relativistic calculation, so this problem appears more remarkably. In this fiscal year, based on the damped-linear response theory considering excitation relaxation, we developed the linear response two-component relativistic time-dependent density functional theory which directly calculates the excitation spectrum of large molecule and implemented it in parallel program. In this method, since the linear equation is solved for each frequency for which the absorption spectrum is desired, a large scale parallelization with respect to the frequency is possible. Then this method can be applied to a high energy excitation spectrum which is difficult to obtain by diagonalization. This Linear-response two-component relativistic TDDFT method was successfully applied to the calculation of the frequency-dependent polarizabilities and the excitation spectra of several molecules containing heavy atoms.

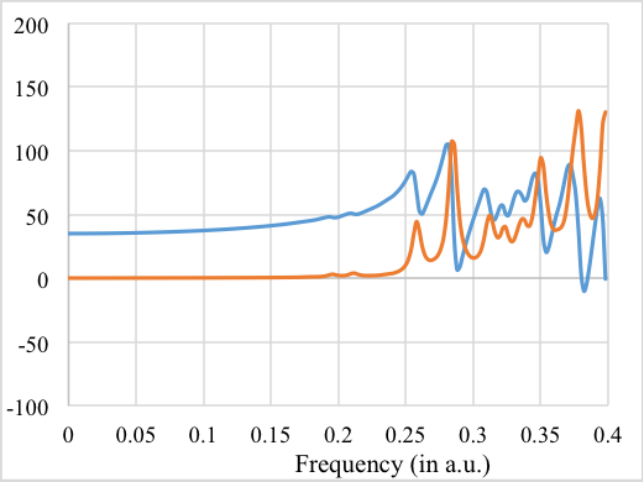


Figure 7.3: Real and imaginary part of dynamical polarizabilities with damping of HI molecule calculated with both scalar and spin?orbit relativistic effects.

7.3.5 Two-component relativistic equation-of-motion coupled-cluster methods for excitation energies and ionization potentials of atoms and molecules

Two-component relativistic equation-of-motion coupled-cluster methods are developed and implemented. Scalar-relativistic and spin-orbit effects are taken into account through a two-component scheme in both HF and correlation calculations. Excitation energies and spin-orbit splittings of atoms and diatomic molecules, and ionization

potentials of OsO_4 are reported. Advantage of the present two-component scheme is illustrated particularly for heavy-element systems.

EOM-CC equation **Two-component spinor**

$$\left(\hat{Q}\bar{H}_N\hat{Q}\hat{R}_k\hat{P}\right)_C = \omega_k\hat{Q}\hat{R}_k\hat{P} \qquad \psi_p = \begin{pmatrix}\psi_p^\alpha \\ \psi_p^\beta\end{pmatrix}$$

7.3.6 New density matrix functional from accurate wavefunction 2RDM analysis

The currently available approximate density functionals used in DFT are not capable of describing the full potential energy curves of molecules. One way of obtaining these curves without resorting to the use of computationally expensive wavefunction methods is to use density matrix functional theory (DMFT). This method has proven to be capable of describing ground state curves for molecules in which a single bond is broken. Recently published functionals which use the concept of geminals are not capable of describing a large part of the correlation energy, but do not completely break down when used for multibond systems. Almost all DMFT functionals that are currently available have been created by some a priori ansatz that generates the second-order reduced density matrix (2RDM) in a direct or indirect way. Instead of generating yet another ansatz very accurate wavefunction 2RDMs (in NO basis) of several small molecules have been analyzed. The results show that a geminal like structure is present, even though it has not been enforced from the onset. Furthermore it is seen that a large part of the missing dynamical correlation is described by multipole-multipole like interactions between the different geminals. The analyis of 2RDMs for multibond systems shows that the original geminal functionals are lacking the appropriate exchange interaction between bond broken electrons that end up on the same fragments. Both of these flaws have been corrected in the newly proposed geminal based ELS-D(ynamical)-M(ultibond) functional. This functional is able to reproduce the results generated by a CASSCF wavefunction that uses the same active space as the ELS-D-M functional (one virtual active orbital for every valence orbital). With the current choice of the active space one can describe 100% of the static correlation, but only 40-50% of the dynamical correlation for the selected molecules.

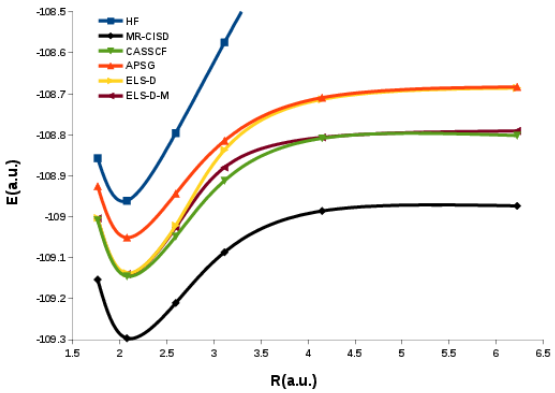
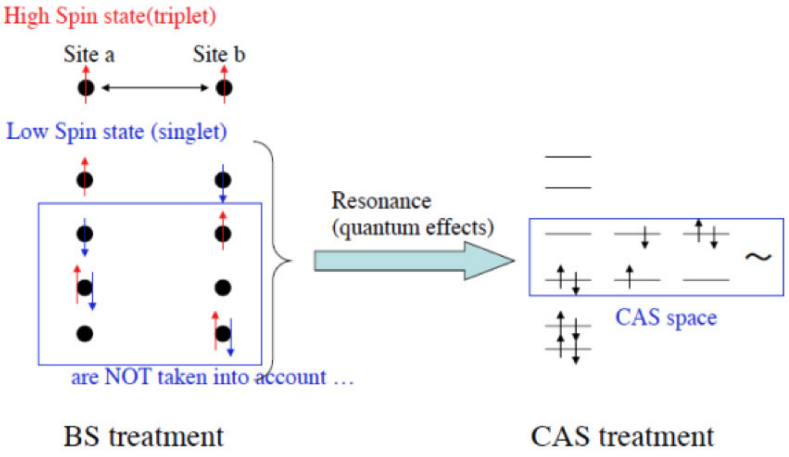


Figure 7.4: N_2 dissociation (aug-cc-pVDZ basis) for various functionals/wavefunctions

7.3.7 UNO DMRG CASCI calculations of effective exchange integrals for *m*-phenylene-bis-methylene spin clusters

Theoretical examinations of the ferromagnetic coupling in the *m*-phenylene-bis-methylene molecule and its oligomer were carried out. These systems are good candidates for exchange-coupled systems to investigate strong electronic correlations. We studied effective exchange integrals (J), which indicated magnetic coupling between interacting spins in these species. First, theoretical calculations based on a broken-symmetry (BS) single-reference (SR) procedure, i.e., the UHF, UMP2, UMP4, UCCSD(T) and UB3LYP methods, were carried out under an SR wave function. From these results, the J value by the UHF method was largely positive because

of the strong ferromagnetic spin polarization (SP) effect. The J value by the UCCSD(T) and UB3LYP methods improved an overestimation problem by correcting the dynamical electronic correlation. Next, magnetic coupling among these spins was studied using the CAS-based method of the symmetry-adapted (SA) multireference (MR) methods procedure. Thus, the UNO DMRG CASCI (UNO = unrestricted natural orbital; DMRG = density matrix renormalized group; CASCI = complete active space configuration interaction) method was mainly employed with a combination of ORCA and BLOCK program codes. DMRG CASCI calculations in valence electron counting (VEC), which included all orbitals to full valence (FV) CI, provided the most reliable result, and supports the UB3LYP method for extended systems.



7.3.8 Implementation of nonadiabatic molecular dynamics simulation by linear-response time-dependent density functional theory

In this fiscal year, we performed research supported by MEXT as "Priority Issue on Post-K computers" (Development of new fundamental technologies for high-efficiency energy creation, conversion/storage, and use). The mission is to design organic photovoltaic solar cells by simulating the power conversion efficiency based on ab initio quantum mechanical methods. However, the theoretical understanding of fundamental reaction mechanisms, i.e., the dynamics of an exciton generated by photo-absorption, is challenging, because the solar cell is a large molecular donor/acceptor system and has many electronic states involved. Therefore, we need computationally efficient methods to simulate photochemical processes on the electronically excited states. To this end, we have developed the Tully's fewest switch surface hopping MD simulation combined with the linear-response TDDFT (LR-TDDFT). The method allows the nonadiabatic transition between states based on the time-dependent Schrodinger equation. We derived numerical nonadiabatic coupling by using the wavefunction overlap and adopted an efficient algorithm reported for the computation of the latter. As a result, the simulation is almost as fast as usual Born-Oppenheimer MD. We interfaced the code with NTChem. Figure 7.5 shows a typical trajectory of the ring-opening reaction of coumarin.

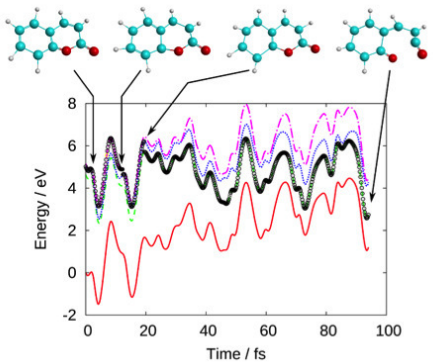


Figure 7.5: Typical trajectory of coumarin starting in S2 ($\pi\pi^*$) state.

7.3.9 Investigation of light induced electron dynamics in molecules

One of the projects of our team is to understand photo chemical process in excited states for examining a scenario of high performance of light-energy conversion. Related to this, we are studying an electron dynamics involved with light-matter, non-adiabatic, and spin-orbit couplings. We constructed a scheme for describing an electron propagation in a time domain based on the real-time TDDFT (RT-TDDFT) with a new additional device on the time integration part. This was implemented into the parallel-version of NTChem. Time dependent Kohn-Sham orbitals were propagated to obtain time dependent properties. Atomic orbital representation was employed. In the test situations of fixed geometry of molecules, we could obtain numerical stability and reliable results on dynamics and photo-absorption spectrum peaks. The latter is not aimed for a realistic model, and in fact compared with the result of the other method, namely, LR-TDDFT code in GAMESS with a primitive basis and exchange-correlation functional. This was intended to check in an orthogonal manner about the correctness of employed time integration, approximations and obtained properties. We formally generalized the Crank-Nicolson scheme for treating non-linear type of Schrodinger equation. The validity and practical feasibility were verified numerically by comparing with the Taylor expansion scheme. For reducing a spectrum range of Hamiltonian, we introduced the concept of time coarse graining for core orbitals having deep energies. This is a time counterpart of the introduction of a pseudo mass for electron employed in the Car-Parinello dynamics. The application to di-keto-pyroro-pyrrole molecule, which is one of organic solar cell material, was successful as shown in Fig. 7.6.

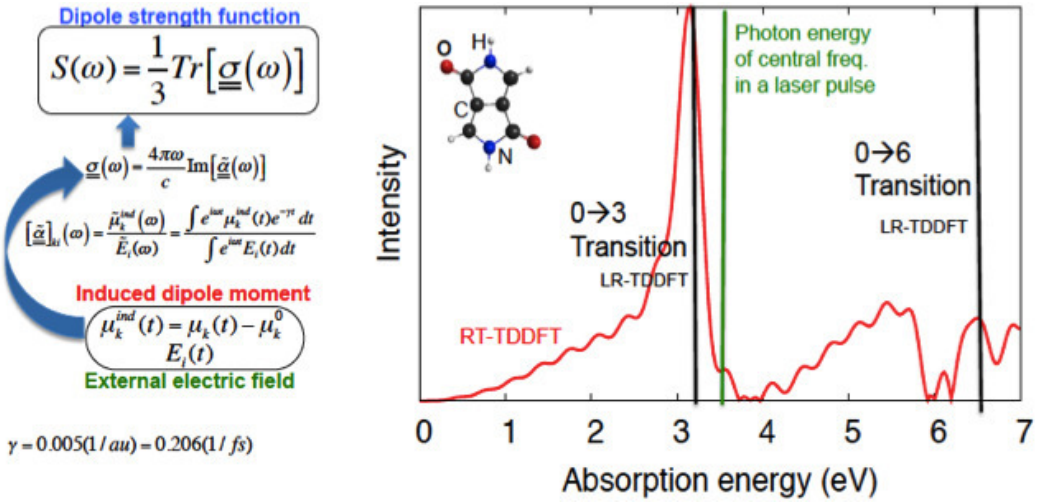
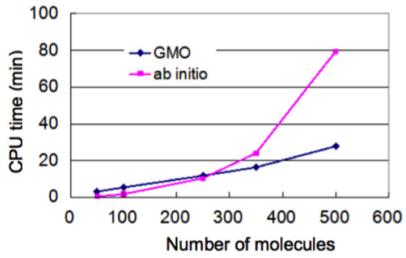


Figure 7.6: Comparison of photo absorption spectrum between RT/LR-TDDFT. Left panel: calculation formula by RT-TDDFT. Right panel: absorption spectrum obtained by using RT-TDDFT (red) and excitation energies obtained from LR-TDDFT (black). The molecular structure is also shown in the inset with the right, upper and front facing directions being X, Y and Z directions. The characteristic time width of light pulse is about 1 fs, the peak strength of light is 0.01 a.u. (3.5×10^{12} W/cm^2) and the central frequency of light is 0.1287 a.u. (corresponding to 3.502 eV). The peak time is 2.42 fs. The polarization direction is parallel to (X,Y,Z) = (1,1,1). The time step is 2 atto second and propagation was carried out till 15 fs. The time dependent properties after 1 fs were used. $0 \rightarrow 3$ and $0 \rightarrow 6$ excitations energies are respectively 3.184 eV and 6.372 eV in LR-TDDFT. Basis function and exchange-correlation functional type are 6-31G and PBE., respectively.

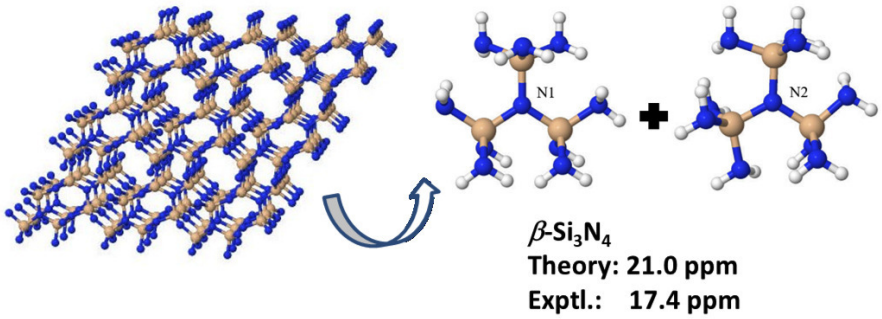
7.3.10 Group molecular orbital approach to solve the Huzinaga subsystem self-consistent-field equations

An algorithm to solve the Huzinaga subsystem self-consistent field equations is proposed using two approximations: a local expansion of subsystem molecular orbitals and a truncation of the projection operator. Test calculations are performed on water and ammonia clusters, and *n*-alkane and poly-glycine. The errors were 2.2 and -0.6 kcal/mol for $(H_2O)_{40}$ and $C_{40}H_{82}$, respectively, at the HF level with the 6-31G basis set.



7.3.11 An extrapolation scheme for solid-state NMR chemical shift calculations

Conventional quantum chemical and solid-state physical approaches include several problems to accurately calculate solid-state nuclear magnetic resonance (NMR) properties. We propose a reliable computational scheme for solid-state NMR chemical shifts using an extrapolation scheme that retains the advantages of these approaches but reduces their disadvantages. Our scheme can satisfactorily yield solid-state NMR magnetic shielding constants. The estimated values have only a small dependence on the low-level density functional theory calculation with the extrapolation scheme. Thus, our approach is efficient because the rough calculation can be performed in the extrapolation scheme.



7.3.12 Theoretical study on power conversion efficiency of organic photocell

We discussed an ideal diode model with hot charge transfer (CT) states to analyze the power conversion efficiency of organic photocell. Organic devices based on blends of conjugated polymers and fullerene derivative have been gathering much attention as promising photovoltaic applications, because of their low production costs, thin and light structures, flexibilities, designs, and so on. However, the power conversion efficiency of organic photocells still remains low compared with inorganic devices. In order to improve their performance, we need to more deeply investigate the mechanism to generate electric currents from photons. The free carrier generation mechanism from sunlight in organic photocell devise composes of four microscopic processes: photon absorption, exciton dissociation, charge transfer, and charge separation. We previously reported the theoretical method to calculate the charge separation process with the hot CT state effect.[T. Shimazaki *et al.*, Phys. Chem. Chem. Phys., **17**, 12538 (2015). J. Chem. Phys., **144**, 234906 (2016).] In the fiscal year 2016, we integrated the CT state mechanism into the diode model, and calculated several device properties of organic photocell device, such as short circuit current, open circuit voltage, and power conversion efficiency. We investigated the influence of the hot CT effect on organic photocell device. Our study showed that the hot CT state and the dimensional effect give strong influences on the device performance as shown in Figure 7.7. The details of our research in last fiscal year were reported in T. Shimazaki *et al.*, Phys. Chem. Chem. Phys., **19**, 12517 (2017).

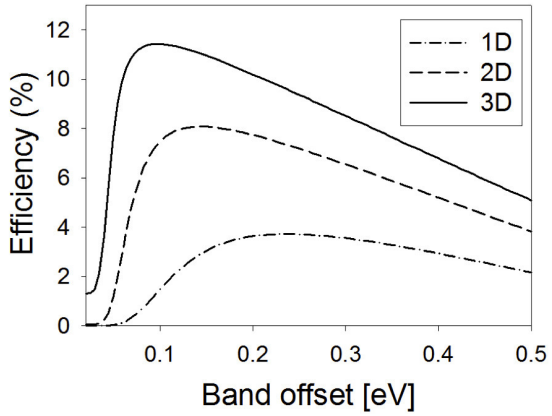
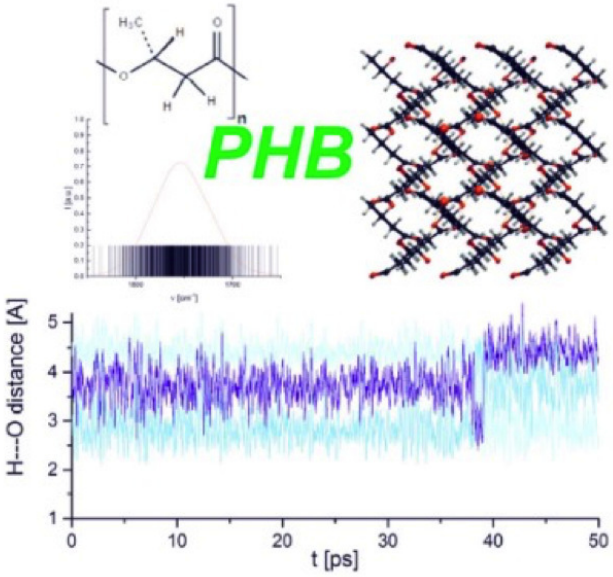


Figure 7.7: Changes of device power conversion efficiency in accordance with band offsets and the dimensional (entropy) effect.

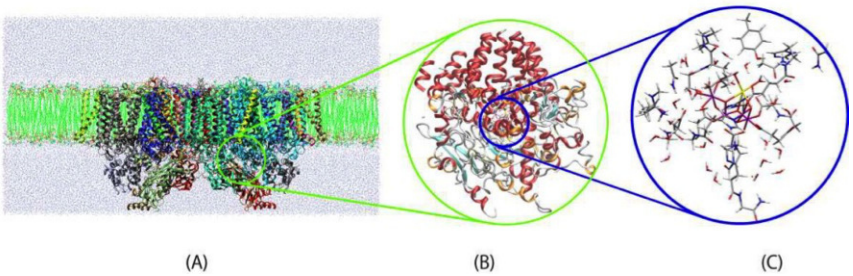
7.3.13 The Born-Oppenheimer molecular simulations of infrared spectra of crystalline poly-(R)-3-hydroxybutyrate with analysis of weak C-HO=C hydrogen bonds

We studied dynamics of week C-HO=C hydrogen bonds of crystalline poly-(R)-3-hydroxybutyrate (PHB) by using Born-Oppenheimer approach as molecular dynamics calculations. The focal point of our study was to rationalize experimental infrared (IR) spectra of PHB by using calculated anharmonic vibrational spectra. The polymeric structure of PHB was determined by the presence of the week hydrogen bonds using BO molecular dynamics. The infrared spectra of PHB were calculated using anharmonic approximation and the time course of the dipole moment function as obtained from the Born-Oppenheimer simulation. Furthermore, we applied the post-molecular dynamics analysis to consider a C=O motion as indirectly involved in the hydrogen bonds. Quantization of the nuclear motion of the oxygens was done to perform detailed analysis of the strength and properties of the C=O bands. We have also shown the dynamics character of the weak hydrogen bond interactions. These interactions, despite in the weak strength, have a great importance in the formation of the polymeric structure of PHB.



7.3.14 Large-scale QM/MM calculations of the $CaMn_4O_5$ cluster in the S_3 state of the oxygen evolving complex of photosystem II. Comparison between water-inserted and no water-inserted structures

Large-scale QM/MM calculations were performed to elucidate the optimized geometrical structure of the $CaMn_4O_5$ cluster with and without water insertion in the S_3 state of the oxygen evolving complex (OEC) of photosystem II (PSII). The left (L)-opened structure was found to be stable under the assumption of no hydroxide anion insertion in the S_3 state, whereas the right (R)-opened structure became more stable if one water molecule is inserted to the Mn_4Ca cluster. The optimized $Mn_a(4)$-$Mn_d(1)$ distance by QM/MM was about 5.0 Å for the S_3 structure without the inserted hydroxide anion, but it is elongated by 0.2-0.3 Å after its insertion. These computational results are discussed in relation to the possible mechanisms of O-O bond formation in the water oxidation by OEC of PSII.



7.4 Schedule and Future Plan

In the next financial year, we will continue to develop new algorithms and improve the parallel efficiency of the NTChem2013 suit of program. For the development of sparse matrix library, we are continuing work on this project by developing new benchmark systems that can both be used to study the performance of our current codes, as well as be used for our future QM/MM investigation. We are developing the distributed memory parallel code for DFT calculation and LR-TDDFT calculation applying this sparse matrix library. The spin-orbit coupling often plays the important role for the unique phenomena of molecules containing heavy elements. We are also developing the distributed memory parallel code of two-component relativistic DFT calculation and LR-TDDFT calculation to account for the spin-orbit interactions explicitly. To further improve the PS method so that we can do fast and efficient calculation on large molecular systems, we are planning to do coding and tuning of related programs in NTChem. We earnestly hope that NTChem will be an important tool leading the way toward a new frontier of computational molecular science.

7.5 Publications

7.5.1 Journal Articles

[1] Tomomi Shimazaki and Takahito Nakajima. "Theoretical Study on Hot Charge-Transfer States and Dimensional Effects of Organic Photocells based on the Ideal Diode Model". In: *Physical Chemistry Chemical Physics* **19** (2017), pp. 12517.

[2] Tomomi Shimazaki, Kazuo Kitaura, Dmitri G. Fedorov, and Takahito Nakajima. "Group molecular orbital approach to solve the Huzinaga subsystem self-consistent-field equations". In: *The Journal of Chemical Physics* **146** (2017), pp. 084109.

[3] Michio Katouda and Takahito Nakajima. "MPI/OpenMP Hybrid Parallel Algorithm for Resolution of Identity Second-Order Møller?Plesset Perturbation Calculation of Analytical Energy Gradient for Massively Parallel Multicore Supercomputers". In: *Journal of Computational Chemistry* **38** (2017), pp. 489-507.

[4] Michio Katouda, Akira Naruse, Yukihiko Hirano, and Takahito Nakajima. "Massively parallel algorithm and implementation of RI-MP2 energy calculation for peta-scale many-core supercomputers". In: *Journal of Computational Chemistry* **37** (2016), pp. 2623-2633.

[5] Tomomi Shimazaki and Takahito Nakajima. "Application of the dielectric-dependent screened exchange potential approach to organic photocell materials". In: *Physical Chemistry Chemical Physics* **18** (2016), pp. 27554.

[6] Tomomi Shimazaki and Takahito Nakajima. "Theoretical study on the cooperative exciton dissociation process based on dimensional and hot charge-transfer state effects in an organic photocell". In: *The Journal of Chemical Physics* **144** (2016), pp. 234906.

[7] Toru Matsui, Yutaka Imamura, Itaru Osaka, Kazuo Takimiya and Takahito Nakajima. "Analyses of Thiophene-Based Donor?Acceptor Semiconducting Polymers toward Designing Optical and Conductive Properties: A Theoretical Perspective". In: *The Journal of Physical Chemistry C* **120** (2016), pp. 8305-8314.

7.5.2 Invited Talks

[8] William Dawson. *Large scale matrix polynomial computation for linear scaling quantum chemistry.* International Workshop on Massively Parallel Programming for Quantum Chemistry and Physics 2017. Jan. 9, 2017.

[9] Keisuke Sawada and Takahito Nakajima. *Fast evaluation of two-electron integrals using pseudospectral methods.* International Workshop on Massively Parallel Programming for Quantum Chemistry and Physics 2017. Jan. 9, 2017.

[10] Michio Katouda and Takahito Nakajima. *Massively parallel implantation of one-component and two-component relativistic electronic structure theories in NTChem software.* RMET2016. Sep. 26, 2016.

[11] Takahito Nakajima. *NTChem: Quantum Chemistry on K Computer.* 12th ICCMSE 2016. Mar. 19, 2016.

7.5.3 Posters and Presentations

[12] Takehiro Yonehara. *Characterization of non-adiabatic electron wave packets in densely quasi-degenerate excited states.* International workshop on numerical methods and simulations for materials design and strongly correlated quantum matters. Mar. 24, 2017.

[13] Keisuke Sawada and Takahito Nakajima. *Fast evaluations of two-electron repulsive integrals using pseudospectral methods.* International workshop on numerical methods and simulations for materials design and strongly correlated quantum matters. Mar. 24, 2017.

[14] Takehiro Yonehara and Takahito Nakajima. *Parallel computation in solving Liouville-von Neumann equation intended for a study on electron dynamics including spin-orbit, laser-matter and nonadiabatic couplings.* 7th AICS International Symposium. Feb. 23, 2017.

[15] Michio Katouda, Akira Naruse, Yukihiko Hirano and Takahito Nakajima. *Massively parallel and multi-GPU implementation of RI-MP2 energy calculations.* 7th AICS International Symposium. Feb. 23, 2017.

[16] Muneaki Kamiya and Tetsuya Taketsugu. *Ab initio excited-state molecular dynamics approach including spin-orbit coupling and nonadiabatic coupling effects: An application to the photodissociation of CH_3I.* The 57th Sanibel Symposium. Feb. 19-24, 2017.

[17] Takehiro Yonehara and Takahito Nakajima. *Non-adiabatic electron dynamics in a chemical process involved with light-matter and spin-orbit couplings.* International Workshop on Massively Parallel Programming for Quantum Chemistry and Physics 2017. Jan. 9, 2017.

Chapter 8

Computational Materials Science Research Team

8.1 Members

- Seiji Yunoki (Team Leader)
- Yuichi Otsuka (Research Scientist)
- Shigetoshi Sota (Research Scientist)
- Hiroshi Ueda (Research Scientist)
- Mohammad Khazaei (Research Scientist)
- Ahamad Ranjbar (Postdoctoral Researcher)
- Akiko Masaki-Kato (Special Postdoctoral Researcher, joint)
- Sandro Sorella (Senior Visiting Scientist)
- Takami Toyama (Senior Visiting Scientist)
- Yutaka Imamura (Visiting Scientist)
- Susumu Yamada (Visiting Scientist)
- Kazuhiro Seki (Visiting Scientist)
- Michele Casula (Visiting Scientist)
- Keiko Matsuoka (Assistant)

8.2 Research Activities

Strongly correlated materials show great promise for next-generation electronic applications. In order to accelerate the development of functional strongly correlated materials, a reliable theory with good predictability is required. However, the strong interactions that take place in this class of materials do not allow us to apply the traditional band theory based on the density functional theory, which played a major role in the advance of todays electronic technology based on semiconductors.

Consequently, we are developing large-scale numerical simulations for strongly correlated quantum systems, including strongly correlated materials, where the many-body interactions are essential to induce novel phenomena and properties. We are interested particularly in the quantum Monte Carlo method, the density matrix renormalization group method, and tensor network method to simulate not only the ground state but also the dynamics (thermodynamics, excitation dynamics, and real time dynamics) that occur between these systems and materials. We have established a platform for advanced research of strongly correlated quantum systems by developing state-of-the-art simulations.

8.3 Research Results and Achievements

8.3.1 Large-scale QMC simulations

We have implemented a highly efficient QMC code based on the auxiliary-filed scheme for lattice fermion systems at zero temperature. Since numerical calculations involved in this formulation are mostly linear algebraic procedure such as matrix-matrix product and numerical orthogonalization, we can take advantage of the highly optimized numerical library on K computer to calculate physical observables with a high degree of accuracy on unprecedentedly large systems.

By using this improved code, we succeeded to clarify the nature of the Mott transition in interacting Dirac fermions in two spatial dimensions. This quantum phase transition is known to belong to the chiral-$SU(2)$ class in terms of the celebrated Gross-Neveu model in the particle physics. Soon after our report on the Mott transition, similar studies have followed focusing on another universality class, the chiral-Z_2 class. Since the universality classes are categorized into three types in the framework of the Gross-Neveu theory, there is then one remaining universality class whose critical exponents are still unknown, at least by an unbiased numerically-exact method, which is the purpose of the research conducted in this year.

The remaining class is the chiral-$U(1)$ class, which describes a scenario that an order parameter for the $U(1)$ symmetry breaking generates a mass gap in the Dirac electrons. To study this type of quantum phase transition, we employ the attractive Hubbard model,

$$H = \sum_{\langle i,j\rangle,\sigma} t_{ij}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + \text{h.c.}\right) - U\sum_{i}\left(n_{i\uparrow} - 1/2\right)\left(n_{i\downarrow} - 1/2\right), \tag{8.1}$$

where $c^{\dagger}_{i\sigma}$ create an electron with spin $\sigma(=\uparrow,\downarrow)$ at site i and $n_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$. The first term represents the kinetic energy coming from transfer integrals $t_{ij} = -|t|e^{\theta_{ij}}$. The attractive interaction measured by U/t drives the system to the s-wave superconducting phase. We study this model on the triangular lattice [Fig. 8.1(a)], to which alternating π-flux is added to construct the Dirac dispersion in the non-interacting limit [Fig. 8.1(b)]. Though being rather artificial, this model is suitable to study the quantum phase transition of the $U(1)$ symmetry breaking by the unbiased large-scale numerical simulations, because the attractive interaction can be studied by our highly improved QMC code without the notorious negative-sign problem even for the non-bipartite lattice.

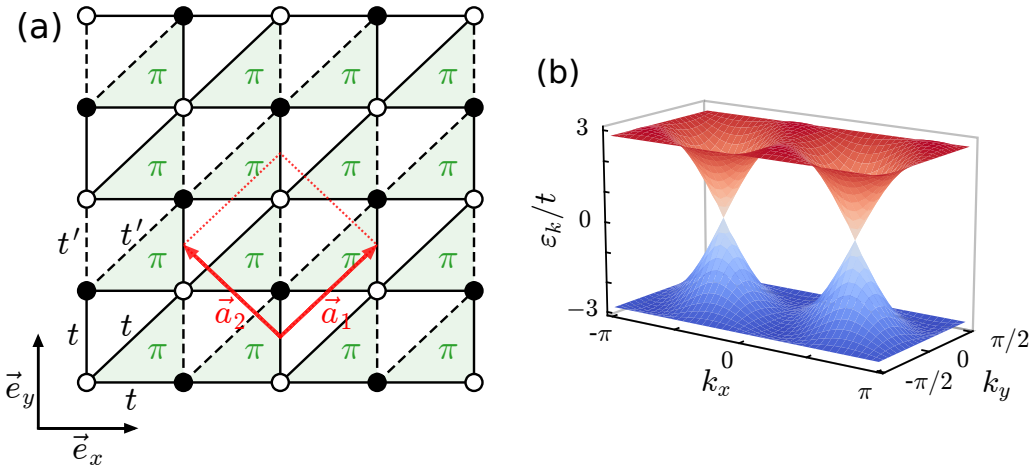


Figure 8.1: (a) Lattice structure of the triangular lattice with alternating π-flux. Each unit cell spanned by the primitive translational vectors (red arrows), $a_1 = (1,1)$ and $a_2 = (-1,1)$, contains two sites. Transfer integral between sites connected by solid (dashed) line is $t = -|t|$ ($t' = -|t|e^{i\pi}$), which results in a magnetic π flux penetrating through each shaded triangle. (b) Energy dispersion in the noninteracting limit ($U/t = 0$). The Fermi level is located at $\varepsilon_k/t = 0$ for half filling.

We calculate the correlation function for the s-wave superconductivity,

$$P_{\text{s}} = \langle \Delta^{\dagger}\Delta + \Delta\Delta^{\dagger}\rangle, \tag{8.2}$$

$$\Delta^{\dagger} = \frac{1}{\sqrt{N_{\text{s}}}}\sum_{l} c^{\dagger}_{l\uparrow}c^{\dagger}_{l\downarrow} \tag{8.3}$$

where N_s denotes the total number of the lattice sites. The QMC simulations are performed on finite size clusters of $(L\vec{e}_x, L\vec{e}_y)$ [Fig. 8.1(a)] with L being linear dimension of the cluster. Depending on whether each cluster has an allowed k point in the discretized reciprocal space, the clusters are divided into two series, $L = 4n$ and $L = 4n + 2$ (n: integer); the former has the k point just at the Dirac point and the latter does not. This difference is reflected in the asymptotic behavior of P_s to the thermodynamics limit (TDL) as a function of $1/L$, as shown in Fig. 8.2. However, it is confirmed that the extrapolated values are consistent for $L = 4n$ and $L = 4n + 2$ and this value corresponds to the s-wave superconductivity order parameter squared, $\Delta_s^2 = \lim_{L\to\infty} P_s/N_s$. By plotting Δ_s as a function of U/t, we determine the critical strength of the interaction, $U_c/t \simeq 7.0$ as well as the corresponding exponent $\beta \simeq 0.7 - 0.8$ assuming $\Delta_s \sim (U/U_c - 1)^\beta$ (see Fig. 8.3).

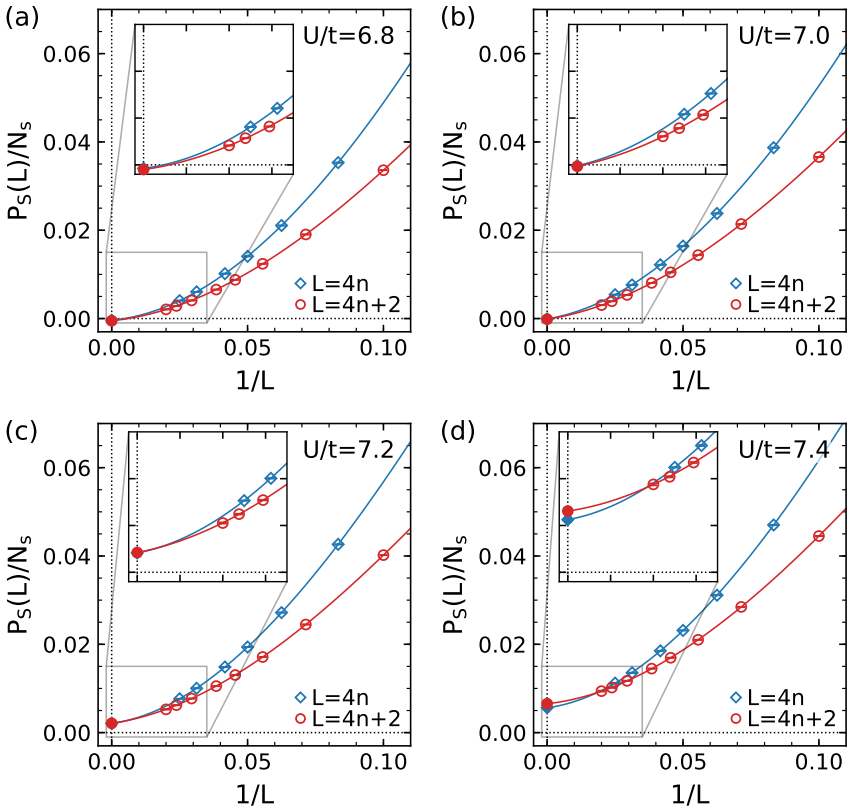


Figure 8.2: Extrapolation of P_s to the thermodynamics limit for four different values of U/t.

Since it is difficult to obtain β with high accuracy by the above-mentioned method, we also try to evaluate β and also the other exponent ν for the correlation length by a more sophisticated manner, finite-size scaling analysis based on Bayesian inference, which has been shown to be reliable in our previous study on the Mott transition. We employ the form of the scaling ansatz,

$$\Delta_s(L, u) \equiv \sqrt{P_s/N_s} = L^{-\beta/\nu} \left(1 + cL^{-\omega}\right) f_\Delta(uL^{1/\nu}), \tag{8.4}$$

where $u = U/U_c - 1$, $f_\Delta(\cdot)$ represents a universal scaling function, and the term proportional to $cL^{-\omega}$ is the lowest order of the correction to the widely-used scaling ansatz. As shown in Fig. 8.4, by collapsing data for $L = 4n$ and $L = 4n + 2$ respectively, we obtain the consistent U_s/t, β, and ν with sufficient accuracy.

Finally, we study the quantum criticality of this transition in the region of the semi-metallic phase. Here, we focus on the density matrix at the maximum distance for each finite-size cluster, $D(r_{\max}) = 1/N_s \sum_r \langle c^\dagger_{r+r_{\max}} c_r \rangle$. Recently, we have noticed that its ratio to those at $U/t = 0$, $Z_L = D(r_{\max})/D^0(r_{\max})$, can be used as a good estimator of the quasiparticle weight, by which we can study a collapse of metallic behavior. The collapse fit of this quantity is shown in Fig.8.5, where U_c/t and ν are consistent with those estimated from P_s, and the other exponent η_Z is estimated as 0.15.

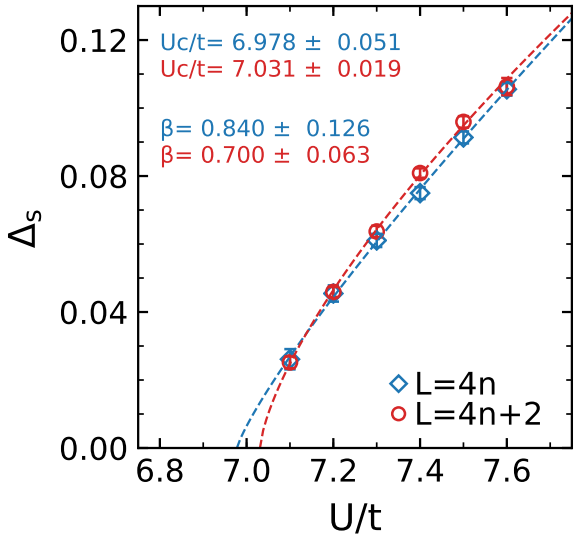


Figure 8.3: Order parameter as a function of U/t estimated from the extrapolations by polynomial fits.

8.3.2 Development of massively parallel density matrix renormalization group program "2D-DMRG"

In order to investigate higher dimensional strongly correlated quantum systems, we have been developing massively parallel density matrix renormalization method (DMRG) program 2D-DMRG. 2D-DMRG can perform not only ground state calculations, but also quantum dynamics such as dynamical DMRG and time-dependent DMRG calculations on higher dimensional systems. We have confirmed that 2D-DMRG shows high performance on the K-computer. The peak ratio of the computational performance of 2D-DMRG is 73.6% at 82,488 nodes, which is 7.8 PFLOPS as the floating-point performance on the K computer.

In this fiscal year, we have expand 2D-DMRG to finite temperature calculations. We have introduced an algorithm where the inner product of a target state corresponds to a partition function at a desired temperature. The target state is calculated recursively using the kernel polynomial method. Figure 8.6 shows the temperature dependence of magnetic susceptibility for the one-dimensional antiferromagnetic Heisenberg model. We can confirm that the 2D-DMRG results are in good agreement with the exact diagonalization results.

8.3.3 Development of massively parallel *ab initio* density matrix renormalization group program "paraDMRG"

We have been developing massively parallel ab-initio DMRG program "paraDMRG". First, we have developed and improved the large scale parallel DMRG method for quantum chemistry. In applications for quantum chemical calculations, the vast number of two-electron integrals strongly limits the number of orbitals L that can be treated in the DMRG method because of explosion of both memory usage and calculation time. In order to overcome this difficulty, we have developed new algorithms and large-scale parallelization for the DMRG method, which allow us to treat orbitals over one hundred on the K computer.

In order to reduce the number of calculating terms in the practical DMRG calculation, we have categorized each operator to gather into each site. Figure 8.7 shows the number of terms calculated in the practical DMRG calculation versus the number of orbitals. A naive algorithm requires the number of the calculating terms $\sim O(L^4)$, but our algorithm scales as $\sim O(L^2)$. This improvement made it possible to treat systems with over 100 orbitals, which significantly exceeds the current limit.

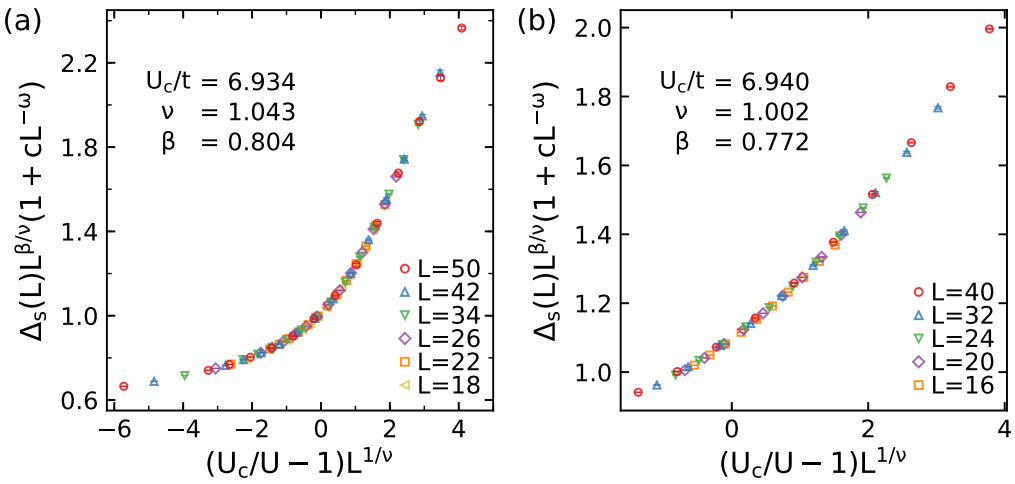


Figure 8.4: Collapse fits of $\Delta_s(L)$ with the correction term.

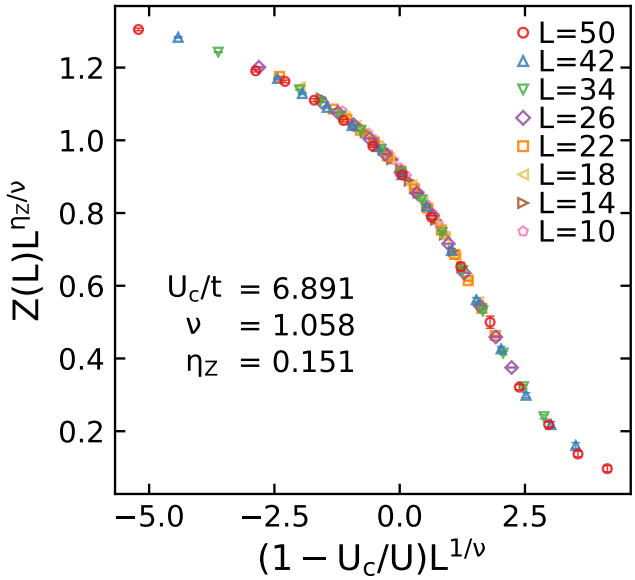


Figure 8.5: Collapse fits of density matrix at maximum distance.

8.3.4 Application of 2D-DMRG to a triangular Kitaev-Heisenberg model

We have studied the Kitaev-Heisenberg (KH) model on a triangular lattice by using our developed 2D-DMRG. The Hamiltonian of the KH model is given as

$$H = \sum_{i,j} (J_K S_i^\gamma S_j^\gamma + J_H \boldsymbol{S}_i \cdot \boldsymbol{S}_j) \tag{8.5}$$

where $\boldsymbol{S}_i$ is a spin-1/2 operator on site i, and γ represents a spin component $\gamma \in x, y, z$. The first term is Kitaev term and the second term is Heisenberg term. The KH model on a triangular lattice has attracted much attention because of its rich phase diagram, including a Z_2-vortex crystal phase, and also because it can describe $Ba_3IrTi_2O_9$, one of candidate compounds of quantum spin liquid with a triangular lattice structure. Since the KH model on a triangular lattice has both geometrical frustration and Kitaev-type frustration that breaks the $SU(2)$ spin symmetry, the quantum effect on the model is expected to be highly nontrivial and interesting.

Here, we have performed the 2D DMRG calculations on a 12×6 site triangular lattice with cylindrical and toroidal boundary conditions. Figure 8.8 shows the obtained magnetic phase diagram. We have also studied the relation among the von Neumann entanglement entropy, the entanglement spectrum, and the phase transitions of the model, and found that the Schmidt gap is much larger than the other gaps among the entanglement

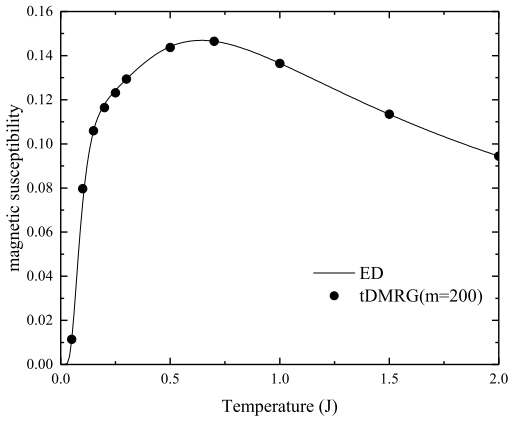


Figure 8.6: The magnetic susceptibility of the antiferromagnetic Heisenberg model on a 16-site chain as a function of temperature. The points shows the finite temperature DMRG results with $m = 200$ and the solid line is the exact diagonalization results.

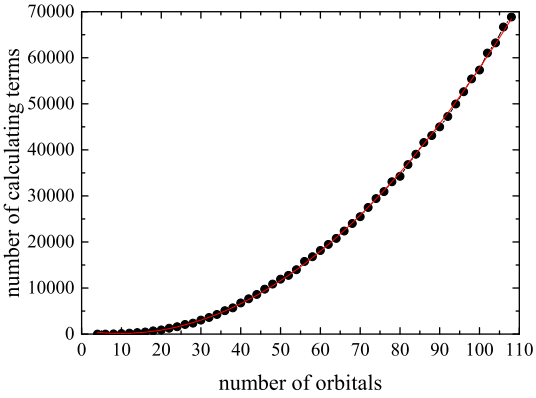


Figure 8.7: The number of calculating terms in the practical ab initio DMRG calculations as a function the number of orbitals. The solid line is a fitting curve using a quadratic function.

levels, and closes at the phase transition points, Therefore, the change in the entanglement structure across the phase transitions is clear in the KH model on the triangular lattice, and this is due to the fact that all the phase transitions are of first order.

8.3.5 Real-space parallelization of infinite-size density matrix renormalization group

We have developed the infinite-size density matrix renormalization group (iDMRG), which is one of the tensor network states (TNS) method, for quasi one-dimensional quantum systems and proposed a parallel algorithm. We have combined the iDMRG for one-dimensional random spin systems with the wave function prediction based of the matrix product state, and have succeeded in proposing a real-space parallelization of iDMRG.

Using this method, we can estimate the physical quantities in the thermodynamic limit directly. We have shown benchmark calculations for a spin-1/2 antiferromagnetic Heisenberg model on a kagome cylinder, where the ground state becomes a spin liquid due to the quantum and geometrical frustrations, and found that the Lanczos iterations of each steps in the parallel iDMRG calculation can be reduced by the prediction and the iDMRG is parallelized efficiently for both shared-memory and distributed memory systems, as shown in Fig. 8.9. The details of this work can be found in arXiv:1606.06790

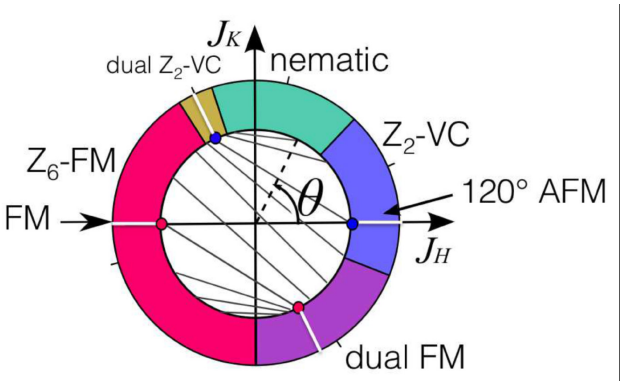


Figure 8.8: Ground state phase diagram of the KH model on the triangular lattice. The circle parametrization of $J_H = \cos\theta$ and $J_K = \sin\theta$ is used. Gray lines inside the inner circle connect the parameter space related by the Klein duality. Filled blue and red circles on the inner circle show parameter points with SU(2) spin-rotational symmetry.

8.4 Schedule and Future Plan

We will continue to develop the quantum Monte Carlo method, the density matrix renormalization group method, and tensor network method to simulate strongly correlated quantum systems, including strongly correlated materials and molecules. In the near future, we are interested in the following subjects.

8.4.1 Fermi liquid or non Fermi liquid in 2D interacting Dirac electrons

Fermi liquid theory is the most fundamental theory of weakly interacting metallic systems. However, this is very often questionable for strongly correlated systems, especially for low-dimensional systems where quantum fluctuations are strong. In fact, it is well known that Fermi liquid theory breaks down in one spatial dimension even when the interactions are weak. The question is what happens in two spatial dimensions. This has been one of the most important questions since the discovery of high-T_c cuprate superconductor in 1986. So far, no definitive answer is available. However, our unprecedentedly large-scale QMC simulations might be able to address this issue numerically. We will plan to improve our QMC program to treat more than 10,000 electrons and simulate interacting Dirac electron in two spatial dimensions with the Hubbard-type on-site interaction and also with the long-range Coulomb interaction.

8.4.2 Time-dependent density matrix renormalization method for quantum annealing and machine learning

We have developed the highly efficient time-dependent DMRG method for higher-dimensional strongly correlated quantum systems. This method is also suitable for quantum annealing simulations. An advantage of our time-dependent DMRG method for quantum annealing is that we can apply this method to any system even if a system is geometrically frustrated, where a QMC method suffers from the negative sign problem. We have already confirmed that the quantum annealing using the time-dependent DMRG method can solve a traveling salesman problem, which is a typical NP-hard problem. The quantum annealing can also be employed for clustering, an unsupervised learning. We will plan to apply our time-dependent DMRG scheme to other fields outside condensed matter physics.

8.4.3 Further development of TNS method

In low-dimensional quantum/classical many-body systems, the TNS method is expected as a versatile method to investigate fascinating phases that the mean field approximation can never predict. However, a sophisticate numerical algorithm for the optimizations of TNS has been demanded because the numerical cost of the optimization is easily increasing with respect to the bond-dimension of tensors. To solve this difficulty, we have focused on the structure, symmetry, and parallelized optimization algorithm of TNS. In general, the accuracy of the expectation value calculated by the TNS method is related to a discarded weight ϵ, which also depends on the bond dimension. The true expectation value can be obtained in the limit of $\epsilon \to 0$, but the extrapolation

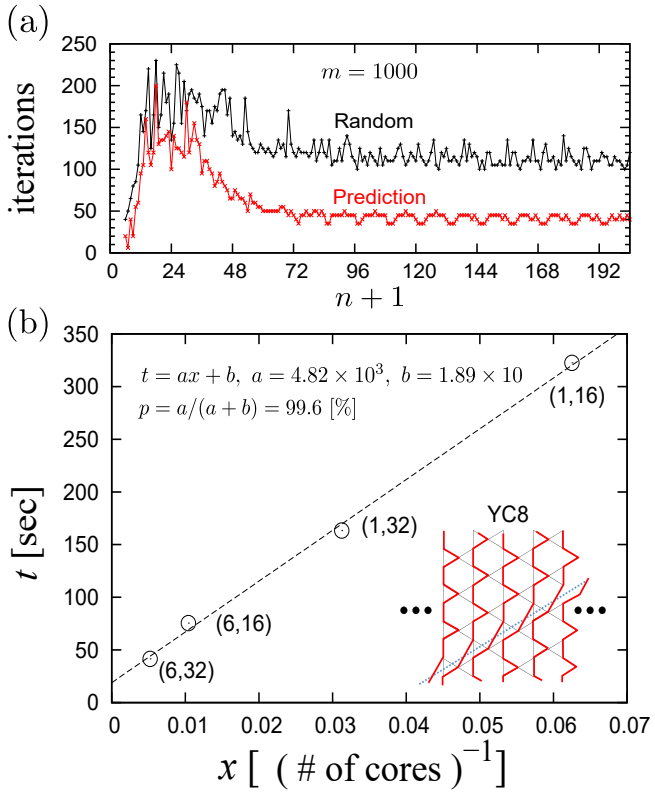


Figure 8.9: (a) The number of iterations for the Lanczos method with/without the wavefunction prediction (+/×) versus the number of iterations for the parallel iDMRG with $m = 1000$, where m is the retained state and determine the bond dimensions of the tensors. (b) Parallel performance of the parallel iDMRG. The computation is performed using 32-core Fujitsu SPARC64 Xlfx 1.975GHz nodes. Each pair of numbers (q, r) beside each circle indicates the number of nodes (q) and threads per node (r) in the hybrid MPI/OpenMP parallel calculations. Calculation time t is defined by the average time of the parallel iDMRG per iteration, where the iteration number n is up to 1200. In the inset, the path of matrix product of our matrix product state is denoted by bold red lines on the YC8.

is unfortunately nontrivial. To estimate the true value, usually, one applies a typical fitting function such as a polynomial function. We believe that this procedure may be sophisticated by use of the knowledge of data science, especially the sparse modeling where we assume large number of parameters for the fitting and the sparseness of the solution. In this sense, it is important to promote the fusion of TNS and data science to investigate the physical property of condensed matters numerically.

8.5 Publications

8.5.1 Journal Articles

[1] Y. Otsuka, S. Yunoki, and S. Sorella, "Universal Quantum Criticality in the Metal-Insulator Transition of Two-Dimensional Interacting Dirac Electrons", Physical Review X **6**, 011029/1-18 (2016).

[2] K. Shinjo, S. Sota, S. Yunoki, K. Totsuka, and T. Tohyama, "Density-matrix renormalization group study of Kitaev-Heisenberg model on the triangular lattice", Journal of the Physical Society of Japan **85**, 114710/1-8 (2016).

[3] K. Seki, T. Shirakawa, Q. Zhang, T. Li, S. Yunoki, "Emergence of massless Dirac quasiparticles in correlated hydrogenated graphene with broken sublattice symmetry", Physical Review B **93**, 155419/1-26 (2016).

[4] T. Shirakawa, S. Yunoki, "Density matrix renormalization group study in energy space for a single-impurity Anderson model and an impurity quantum phase transition", Physical Review B **93**, 205124/1-17 (2016).

[5] M. Khazaei, A. Ranjbar, M. Ghorbani-Asl, M. Arai, T. Sasaki, Y. Liang, S. Yunoki, "Nearly free electron states in MXenes", Physical Review B **93**, 205125/1-10 (2016).

[6] K. Seki, S. Yunoki, "Brillouin-zone integration scheme for many-body density of states: Tetrahedron method combined with cluster perturbation theory", Physical Review B **93**, 245115/1-11 (2016).

[7] Y. Kawasugi, K. Seki, Y. Edagawa, Y. Sato, J. Pu, T. Takenobu, S. Yunoki, H. M. Yamamoto, R. Kato, "Electron-hole doping asymmetry of Fermi surface reconstructed in a simple Mott insulator", Nature Communications **7**, 12356/1-8 (2016).

[8] A. Yamasaki, H. Fujiwara, S. Tachibana, D. Iwasaki, Y. Higashino, C. Yoshimi, K. Nakagawa, Y. Nakatani, K. Yamagami, H. Aratani, O. Kirilmaz, M. Sing, R. Claessen, H. Watanabe, T. Shirakawa, S. Yunoki, A. Naitoh, K. Takase, J. Matsuno, H. Takagi, A. Sekiyama, Y. Saitoh, "Three-dimensional electronic structures and the metal-insulator transition in Ruddlesden-Popper iridates", Physical Review B **94**, 115103/1-10 (2016).

[9] M. Khazaei, A. Ranjbar, M. Arai, S. Yunoki, "Topological insulators in the ordered double transition metals $M'_2M''C_2$ MXenes (M′=Mo, W; M″=Ti, Zr, Hf)", Physical Review B **94**, 125152/1-9 (2016).

[10] Q. Cui, J.-G. Cheng, W. Fan, A. E. Taylor, S. Calder, M. A. McGuire, J.-Q. Yan, D. Meyers, X. Li, Y. Q. Cai, Y. Y. Jiao, Y. Choi, D. Haskel, H. Gotou, Y. Uwatoko, J. Chakhalian, A. D. Christianson, S. Yunoki, J. B. Goodenough, J.-S. Zhou, "Slater insulator in iridate perovskites with strong spin-orbit coupling", Physical Review Letters **117**, 176603/1-6 (2016).

[11] B. H. Kim, T. Shirakawa, S. Yunoki, "From a quasimolecular band insulator to a relativistic Mott insulator in t_{2g}^5 systems with a honeycomb lattice structure", Physical Review Letters **117**, 187201/1-6 (2016).

[12] Y. Kawasugi, K. Seki, Y. Edagawa, Y. Sato, J. Pu, T. Takenobu, S. Yunoki, H. M. Yamamoto, and R. Kato, "Simultaneous enhancement of conductivity and Seebeck coefficient in an organic Mott transistor", Applied Physics Letter **109**, 233301/1-4 (2016).

8.5.2 Posters and Presentations

[13] S. Yunoki, "Quantum criticality of the metal-insulator transition and possible spin liquid in 2D Hubbard models", The 2nd Conference on Condensed Matter Physics, July 20-22 (2016), Nanjing (China). [Invited]

[14] S. Yunoki, "Microscopic model study of strongly correlated 5d transition metal Ir oxides", IUMRS 2016 Symposium Materials Simulation, Computation and Design, October 21-24 (2016), Qingdao (China). [Invited]

[15] S. Yunoki, "Metal-insulator transition in 2D interacting Dirac electrons", Chiral Matter from Quarks to Dirac semimetals, December 5-8 (2016), Wako (Japan). [Invited]

[16] S. Yunoki, "Emergence of massless Dirac quasiparticles in correlated hydrogenated graphene with broken sublattice symmetry", The 11th Anniversary General Meeting of Asian Consortium on Computational Materials Science (ACCMS), November 19-21 (2016) Sendai (Japan). [Invited]

[17] S. Yunoki, "Spin dynamics in two-dimensional S=1/2 antiferromagnets – fate of single magnon excitations –", The 10th International Conference on Computational Physics (ICCP10), January 16-20 (2017), Macao (China). [Invited]

[18] Y. Otsuka, S. Yunoki, and S. Sorella, "Universal quantum criticality in two-dimensional interacting Dirac electrons", The 6th AICS international symposium, Kobe Japan, February 2016. [Poster]

[19] Y. Otsuka, S. Yunoki, and S. Sorella, "Universal quantum criticality in Hubbard models with massless Dirac dispersion", American Physical Society March Meeting 2016, Baltimore USA, March 2016 [Oral]

[20] S. Sota, S. Yunoki, and T. Tohyama, "DMRG study of magnetic order and phase transition between triangular and honeycomb lattice in Kitaev-Heisenberg model", 2016 Autumn Meeting, 16aPS-65, 2016/9, Kanazawa. [Poster]

[21] S. Sota, "Novel quantum phases induced by spin-orbit interaction and spin frustration in triangular spin models", The Third Project Report Meeting, C-20, 2016/10, Shinagawa. [Poster]

[22] S. Sota, "Quantum dynamics of cold atoms on optical lattice", The Third Project Report Meeting, H-2, 2016/10, Shinagawa. [Poster]

[23] S. Sota, T. Shirakawa, S. Yunoki, and T. Tohyama, "Development of time-dependent DMRG method using kernel polynomial method and its application to spin S=1/2 Heisenberg model", The second CDMSI symposium, 2016/12, Kashiwa. [Poster]

[24] S. Sota, "Massively parallel density matrix renormalization group study of two-dimensional systems", International Workshop on Massively Parallel Programming for Quantum Chemistry and Physics 2017, 2017/1, Kobe. [Invited]

[25] S. Sota, T. Shirakawa, S. Yunoki, and T. Tohyama, "Time-dependent DMRG study of non-equilibrium quantum dynamics on two-dimensional Heisenberg model", The 72nd Annual Meeting, 20aC-PS-5, 2017/3, Toyonaka. [Poster]

[26] S. Sota, "Time dependent DMRG method and its application to quantum annealing", 2nd Kobe workshop for material design on strongly correlated electrons in molecules and materials, 2017/3, Kobe. [Poster]

[27] H. Ueda, "Real-space parallel infinite-size density matrix renormalization group", International Workshop on Tensor Networks and Quantum Many-Body Problems (TNQMP2016), 2016/06/27, Kashiwa, Japan. [Invited]

[28] H. Ueda, "Real-space parallelization for infinite-size density matrix renormalization group", Fourth Workshop on Tensor Network States: Algorithms and Applications, 2016/12/12, Hsinchu, Taiwan. [Invited]

[29] H. Ueda, "Wavefunction predictions based on tensor network algorithms in quantum spin systems", 6th Joint Laboratory for Extreme Scale Computing Workshop, 2016/12/01, Kobe, Japan. [Oral]

[30] H. Ueda, "Algorithm for large scale calculations of real-space parallel infinite-size density matrix renormalization group", The 2016 Autumn JPS Meeting, 2016/09/14, Kanazawa, Japan. [Oral]

[31] M. Khazaei and S. Yunoki, "Electronic properties of MXenes and their possible, applications of MXenes", The 11th General Meeting of Asian Consortium on Computational Materials Science-Virtual Organization (ACCMS-VO), Sendai, Tohoku University, 19-21 December, 2016. [Oral]

[32] A. Ranjbar and S. Yunoki, "Structural, electronic, and magnetic properties of Cr_2AX (A=Al, Ge, Ga; X=C, N, B) MAX phases", The 11th General Meeting of Asian Consortium on Computational Materials Science-Virtual Organization (ACCMS-VO), Sendai, Tohoku University, 19-21 December, 2016. [Oral]

[33] M. Khazaei, A. Ranjbar, and S. Yunoki, "MXenes: promising platforms for fundamental research and device application", 2nd Kobe workshop for material design on strongly correlated electrons in molecules and materials, March 22-25, 2017 Kobe, Japan. [Poster]

[34] A. Ranjbar, M. Khazaei, and S. Yunoki, "Structural, electronic, and magnetic properties of Cr_2AX (A=Al, Ge, Ga; X=C, N, B) MAX phases", 2nd Kobe workshop for material design on strongly correlated electrons in molecules and materials, March 22-25, 2017 Kobe, Japan. [Poster]

8.5.3 Patents and Deliverables

[35] S. Sota, T. Tohyama, and S. Yunoki, massively parallel DMRG program "2D-DMRG", AICS software.

Chapter 9

Computational Biophysics Research Team

9.1 Members

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9.2 Research Activities

We mainly have developed GENESIS (Generalized Ensemble Simulation system) for molecular dynamics simulations. GENESIS is highly parallelized on K and other massively parallel supercomputers, and has a lot of enhanced conformational sampling methods. In March, 2014, we provided the first pre-released version of GENESIS as free software under the license of GPLv2 on the team website. In this fiscal year, we updated GENESIS with better performance and with advanced algorithms. We also added new functions to enlarge the application range of GENESIS. These updates are released as GENESIS 1.1.

9.3 Research Results and Achievements

9.3.1 Release of GENESIS 1.1

GENESIS is aimed at enlarging system size and simulation time by adopting highly parallelized schemes and enhanced conformational sampling algorithms. We have developed efficient algorithms and implemented functions after release of GENESIS 1.0. The new version, GENESIS 1.1, contains several significant updates of functions, models, and computations. The all-atom and physical-based/structure-based coarse-grained potential energy functions used in AMBER and GROMACS packages now become available in addition to CHARMM energy functions. The performance of GENESIS 1.1 has been improved compared to the previous version by (1) introducing multiple time step integration based on reversible reference system propagator algorithm (RESPA), (2) enabling GPUs on hybrid (CPU+GPU) computers, (3) enabling mixed-precision floating points. GENESIS 1.1 has better performance than GENESIS 1.0, showing good parallel scaling up to 16000 nodes for a 28.8 M system (Figure 9.1). The new version of GENESIS also has more enhanced sampling calculations, including the string method and replica-exchange umbrella sampling with off-lattice collective variables. The new features of the updates increase the usefulness and power of GENESIS for modeling and simulation in biological research.

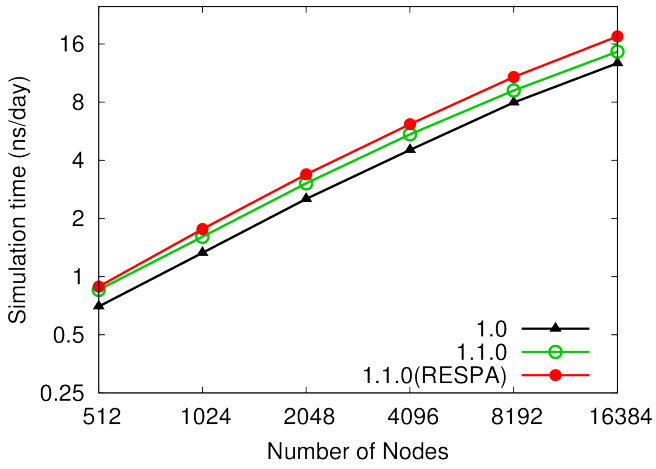

Figure 9.1: Benchmark of GENESIS on K computer (28.8 M atoms system)

9.3.2 Increasing of parallel efficiency of GENESIS by multiple program/multiple (MPMD) data scheme

To increase the parallel efficiency of MD, we have developed multiple program/multiple data (MPMD) scheme which separates processors responsible for real space and reciprocal space calculations. The new method shows better performance for very large number of processors. It also increases the available number of processors. Based on this, we developed multiple time step integration where communication-intensive part is skipped regularly during MD simulations. The new method is tested on K computer, and 60 % speed up is investigated for a 28.8 M atoms system (Figure 9.2).

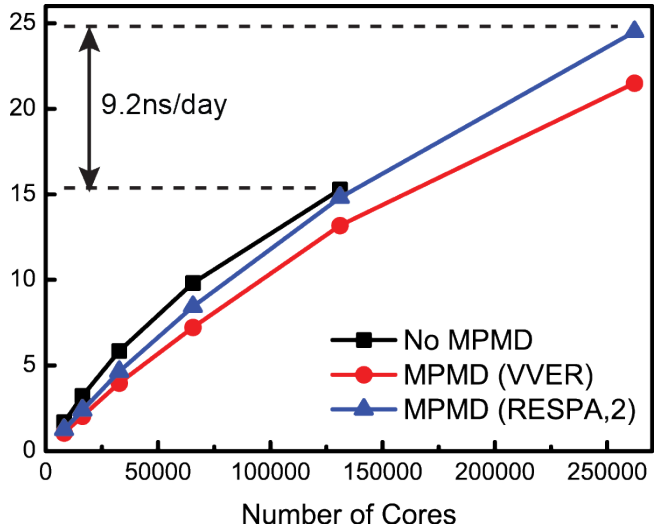

Figure 9.2: Benchmark of MPMD on K computer (28.8 M atoms system)

9.3.3 Machine learing approach for combining single-molecule experiments and simulations

Single-molecule experiment and molecular dynamics (MD) simulation are indispensable tools for investigating protein conformational dynamics. The former provides single-molecule time-series data, such as donor-acceptor distances, while the latter gives atomistic motions, though often biased by model parameters. We have developed a machine learning algorithm to link the two approaches and construct an atomically detailed and experimentally consistent model of protein dynamics. It is applied to the folding dynamics of a dye-labeled WW domain of the formin-binding protein1. MD simulations over 400 microseconds led to an initial Markov state model, which was then refined using single-molecule F 日 rster resonance energy transfer (FRET) time-series data through hidden Markov modeling. The refined model reproduces experimental FRET efficiency and features hairpin 1 in the transition-state ensemble, consistent with mutation experiments. Our machine learning process provides a general framework applicable to investigating conformational transitions in other proteins (Figure /reffig:fig3).

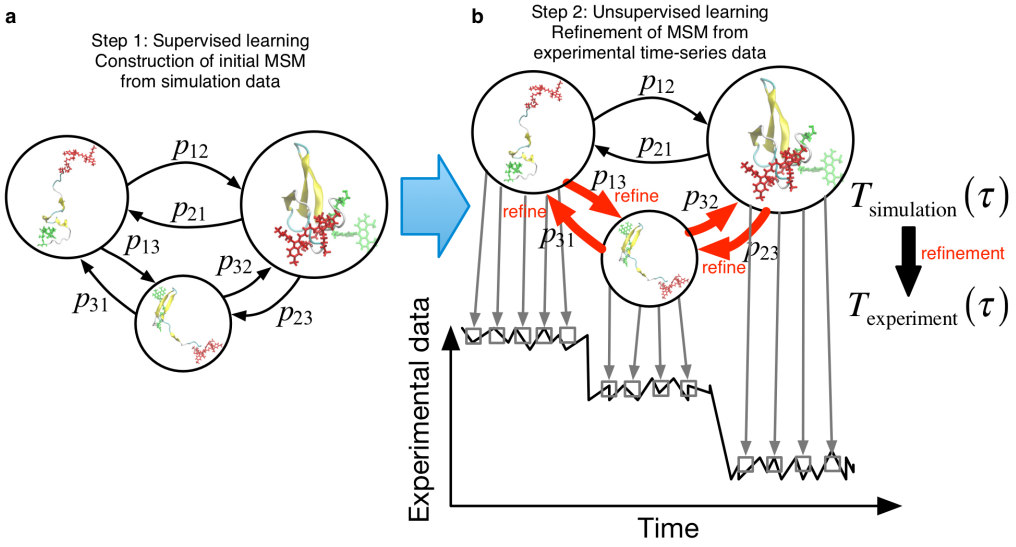

Figure 9.3: Schematic of our semi-supervised learning approach. (a) Current approach comprises two steps: As the first step, an initial Markov State Model data is constructed only from simulation data by simpley counting transitions between conformational states. (b) In the second step, transition probabilities (depicted with arrows) are updated through the unsupervised learning from experimental time-series data

9.3.4 Development of generalized replica-exchange with solute tempering (gREST)

Conformational search is still one of the important problems in molecular dynamics (MD) simulations of biomolecules. We developed a new method for the conformational search, which we call gREST (generalized replica exchange with solute tempering). This method allows us flexible separation of solute and solvent energy terms, which significantly reduces the required number of replicas in comparison with conventional REST. We applied this method to a vast conformation search involving folding events of TrpCage mini-protein. Our new method successfully found the folded state in comparable timescale as conventional REST, while the computation cost was half of the conventional one. The free energy map also converged rapidly in gREST due to the decreased number of replicas and more efficient random walk performance in parameter space (Figure /ref-fig:fig4).

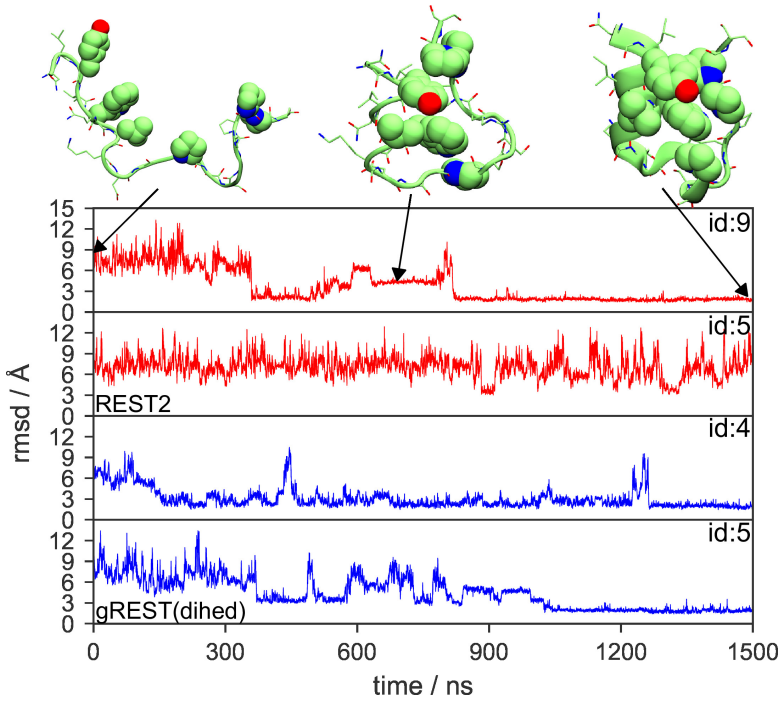

Figure 9.4: RMSD time series of TrpCage from conventional REST and gREST trajectories. The initial structure (top-left) was unfolded state. Ten and five replicas were employed for conventional REST (REST2) and gREST, respectively

9.3.5 Computational modeling of the ATP-bound outward-facing form of a heme importer

Bacteria infected on a human body take iron as a nutrient from the host in the form of heme iron. As heme iron cannot pass through intact cell membrane of bacteria, bacteria prepare unique machine in its cell membrane, and efficiently absorb heme iron. This molecular machine is called heme importer. Heme importer belongs to the large family of type-II ATP-binding cassette (ABC) transporter. Transport of heme across the cell membrane involves large and global conformational changes of the protein during which two ATPs are consumed. Type-II ABC transporter to which heme importer belongs is believed to follow the alternating access mechanism where the transporter can alternate between an inward-facing (IF) form and an outward-facing (OF) one. Recently, crystal structures of bacterial heme importer in the ATP-free inward-facing form have been solved. Based on the structures and biochemical experiments, a molecular mechanism for heme transport cycle was proposed. In this study, computational modeling approach was adopted to model the ATP-bound OF form of the heme importer and thereby complement the molecular model of the transport cycle. An iterative remodeling approach yielded a structurally stable atomistic model and revealed a gating mechanism for the OF form (Figure /reffig:fig5).

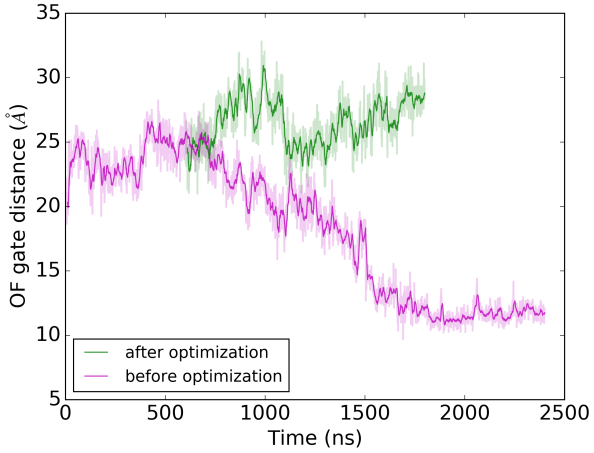

Figure 9.5: Gating mechanism of OF

9.4 Schedule and Future Plan

Until now, GENESIS has been optimized considering only a few computational platforms: K, Intel Sandy Bridge, and NVIDIA Tesla GPU. From this fiscal year, we will consider optimizations for recently developed CPU and GPU architectures, including Intel Haswell/Broadwell/KNL, postK, and NVIDIA Pascal GPU. We will also introduce multi kernels according to each platform. We will further improve the enhanced sampling method for more precise free energy evaluation by merging generalized replica-exchanged with solute-tempering (gREST) into free energy perturbation (FEP).

9.5 Publications

9.5.1 Journal Articles

[1] Jaewoon Jung, Akira Naruse, Chigusa Kobayashi, and Yuji Sugita., "Graphics Processing Unit Acceleration and Parallelization of GENESIS for Large-Scale Molecular Dynamics Simulations.", J. Chem. Theory Comput., 12, 4947 - 4958 (2016).
[2] Isseki Yu, Takaharu Mori, Tadashi Ando, Ryuhei Harada, Jaewoon Jung, Yuji Sugita, Michael Feig, "Biomolecular interactions modulate macromolecular structure and dynamics in atomistic model of a bacterial cytoplasm.", eLife, 5, e19274 (2016).
[3] Jaewoon Jung and Yuji Sugita, "Multiple program/multiple data molecular dynamics method with multiple time step integrator for large biological systems", J. Comput. Chem. 38, 1410 – 1418 (2017)
[4] Osamu Miyashita, Chigusa Kobayashi, Takaharu Mori, Yuji Sugita, and Florence Tama, "Flexible fitting to cyro-EM density map using ensemble molecular dynamics simulations", J. Comput. Chem., 38, 1447 – 1461 (2017)

9.5.2 Book

[5] Jaewoon Jung and Yuji Sugita, HPC Technology for Computational Science 1. Chapter 9 (Osaka Univeristy press) (written in Japanese)

9.5.3 Conference Papers

9.5.4 Invited Talks

[6] Jaewoon Jung and Yuji Sugita, "Efficient Parallelization of Molecular Dynamics on Hybrid CPU/GPU Supercomputers", 2016 GTC Conference, San Jose Convention Center, April 4 – 7 (2016)
[7] Yuji Sugita, "Two-step Proton Transfer Mechanism in the Outward-Facing Form of MATE Multidrug Transporter", IAS Focused Program on Molecular Machines of Life: Simulation Meets Experiments, Hong Kong University of Science and Technology, May 26 (2016)

[8] Yuji Sugita, "Membrane protein dynamics and folding by enhanced conformational sampling", Symposium on Free Energy Landscape of Protein Folding and Dynamics by Simulations based on Enhanced Conformational Sampling Algorithms, Nagoya University, August 6 (2016)
[9] Yuji Sugita, "Enhanced conformational sampling methods for conformational dynamics of proteins, membranes, and N-glycans", International Workshop on Frontiers in Molecular Biophysics, Shanghai, China, July 23 – 25 (2016)
[10] Yuji Sugita, "Enhanced conformational sampling methods for membrane protein folding and dynamics", 4th International Conference on Molecular Simulations 2016 (ICMS2016), Shanghai, October 23 – 26 (2016)
[11] Yuji Sugita, "In-vivo Macromolecular Crowding Effects", Telluride Summer Conference on Protein and Peptide Dynamics in Cellular Environments, June 27 – July 1 (2016)
[12] Chigusa Kobayashi, Yasuhiro Matsunaga, Jaewoon Jung, and Yuji Sugita, "Multi-resolution simulation method for reaction mechanism analsysis of large scale structural change of P-type ATPase", The 89th Annual meeting of the Japanese Biochemical Society, Sendai, Japan, September 26 (2016) (in Japanese)
[13] Yasuhiro Matsunaga, "Functional dynamics of AcrB multidrug transporter by string method", The 10th Keihan KEIHANNA Seminar, Kyoto University, Japan, March 22 (2017)
[14] Yasuhiro Matsunaga, "Drug extrusion mechanism of the multidrug transport AcrB studied by molecular dynamics simulation", The 97th Annual meeting of Chemical Socieity of Japan, Keio Hiyoshi Campus, Japan, March 18 (2017)
[15] Yasuhiro Matsunaga, "Markov state modeling of protein folding dynamics by combining single-molecule experiments and simulations", Simulations Encounter with Data Science in Institute of Statistical Mathematics, Tokyo, March 9 – 11 (2017)
[16] Yasuhiro Matsunaga, "A method for searching reaction degrees of freedom in protein structure change", The 10th Molecular Simulation School-from basic to applied, Okazaki, Japan, October 19 (2016) (in Japanese)
[17] Yasuhiro Matsunaga, "Data assimilation in biomolecules", RIKEN Data assimilation workshop, Kobe, Japan, October 14 (2016) (in Japanese)
[18] Yasuhiro Matsunaga, "Analysis of sinlge molecule FRET data and protein dynamics by molecular dynamics simulation", The 16th Annual meeting of the Japanese Protein Science Association: Symposium of Young Scientist Awards, Fukuoka, June 7 – 9 (2016) (in Japanese)
[19] Yasuhiro Matsunaga, "Analysis of single molecule FRET data and protein dynamics by molecular dynamics simulation", The 16th Annual meeting of the Japanese Protein Science Association: Workshop "Sparse Modeling of Life Molecular Measurements", Fukuoka, Japan, June 7 – 9 (2016) (in Japanese)

9.5.5 Posters and Presentations

[20] Chigusa Kobayashi, Yasuhiro Matsunaga, Jaewoon Jung, and Yuji Sugita, "Analysis of reaction path of calcium ion pump by computer simulation", The 42th Annual meeting of Japanese Bioenergetics Group, Nagoya, Japan, Dec. 20 (in Japanese)
[21] Chigusa Kobayashi, Yasuhiro Matsunaga, Jaewoon Jung, and Yuji Sugita, "Molecular dyanmics simulations for reaction with large conformational changes in biological system", The 7th AICS International Symposium, Feb. 23 (2017)
[22] Jaewoon Jung and Yuji Sugita, "Multiple program/multiple data molecular dynamics method with multiple time step integrator for large biological systems", The 30th Annual meeting of Molecular Simulation Society, Osaka, Japan, Nov. 30 – Dec. 2 (2016)
[23] Motoshi Kamiya and Yuji Sugita, "In silico folding simulation of Trp-cage using the REST method and its variants", The 54th Annual meeting of the Japanese Biophysical Society, Tsukuba, Japan, Nov. 26 (2016)
[24] Koichi Tamura and Shigehiko Hayashi, "Deciphering alternating access mechanism of a Mitochondrial ADP/ATP Membrane Transporter with Atomistic Simulations", The 54th Annual meeting of the Japanese Biophysical Society, Tsukuba, Japan, Nov. 25 (2016)

9.5.6 Patents and Deliverables

[25] Generalized-Ensemble SImulation System (GENESIS) is released. https://aics.riken.jp/labs/cbrt/

Chapter 10

Particle Simulator Research Team

10.1 Members

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10.2 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 be divided into grid-based and particle-based methods. 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

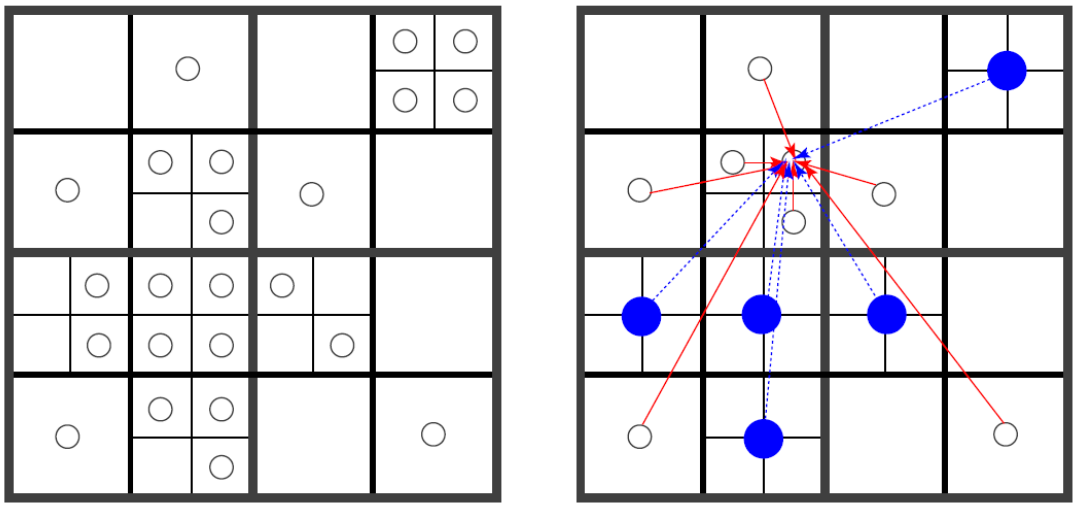

Figure 10.1: Basic idea of tree algorithm

the error comes from the high velocity, while that error would be transferred to internal energy of the fluid element which is much smaller than that of the kinetic motion.

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

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

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

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

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

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

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

Our goal is to develop a "universal" software that can be applied to a variety of problems whose scales are vastly different. In designing such universal software, it is important to ensure that it runs efficiently on highly parallel computers such as the K computer. Achieving a good load balance with particle-based simulation is a difficult task, since using a regular spatial decomposition method causes severe load imbalance, though this

works well for grid-based software. Consequently, we have developed an adaptive decomposition method that is designed to work in a way that the calculation time on each node is almost the same, resulting in near-optimal load balance.

The strategy to develop such a universal software is as follows.

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

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

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

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

10.3 Research Results and Achievements

As we stated in section 1, 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.

10.3.1 High-performance gravitational N-body solver.

We use the TreePM algorithm as the basic method for the evaluation of gravitational interaction between particles. TreePM is a combination of the tree method and the P^3M (particle-particle particle-mesh) scheme. Figure 1 shows the basic idea of the tree algorithm. The space is divided into a hierarchical octree structure (quadtree in the figure). Division is stopped when a cell contains one or no particle. When we calculate the force on a particle, we evaluate the force from a group of particles, with size larger for more distant particles. In this way, we can reduce the calculation cost from O(N2) to O(N log N).

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

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

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

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

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

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

10.3.2 Particle Simulation Platform.

In FY 2014, We have completed and released Version 1.0 of the particle simulation platform, which we call FDPS (Framework for Developing Particle Simulator). In FY 2015, we have applied a number of improvements to FDPS.

The basic idea of FDPS is that the application developer (or the user) specified the way the particles interact with each other, and the rest is taken care by FDPS. Here, "the rest" includes domain decomposition and re-distribution of particles, evaluation of interactions between particles, including those in different domains (different MPI processes, for example).

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

The base layer of FDPS offers the domain decomposition based on the recursive multisection algorithm, with arbitrary weighting function for the load balancing. It also offers the parallel implementation of interaction calculation between particles.

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

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

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

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

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

In FY 2015, we have extended FDPS in several important directions. The first one is the improvement of the strong scaling. The algorithm used for the domain decomposition contains one serial bottleneck. The "sampling" algorithm used in FDPS 1.0 works well only when the average number of particles per MPI process is significantly larger than the total number of MPI processes. We developed a new parallel algorithm, in which $O(p^{1/3}$ MPI processes are used to decompose the computational domain. Here p is the total number of MPI processes. Thus now the requirement for the number of particle is relaxed from larger than p to larger than $p^{2/3}$.

Now we can achieve pretty good performance for around 1 billion particles, on the full nodes of K computer. Previously we need near 100 billion particle to achieve good efficiency.

The second one is the addition of new interface method to interaction calculation function, which allows efficient use of accelerator hardware such as GPGPU or Intel MIC. In order to achieve high performance on accelerators, it is important to pass a large chunk of work at one time. In order to achieve this goal, in the current version of FDPS the CPU creates the list of multiple interaction lists, and send all of them at once so that the overhead of the initialization of the accelerator would not become a bottleneck. This interface has been tested on NVIDIA GPGPUs as well as the PEZY-SC processor.

In FY 2016, we have released FDPS 3.0. The most important new feature of this release is the interface to application programs written in Fortran. FDPS itself is implemented using C++. The reason why we adopted C++ is to use its "template" functions. Using templates, we can write library functions which accept user-defined data types as template arguments. This means we can effectively generate "specialized" libraries for user-specified particle data types, without knowing the data types beforehand.

However, a number of researchers in the HPC fields are using Fortran, because of various reasons. Therefore, if we can somehow provide the interface between FDPS and Fortran-written user programs, that would certainly help the HPC community.

Fortunately, Fortran standards after Fortran 2003 supports "iso_c_binding" which defines how Fortran (sub) programs can inter-operate with C functions. Using this functionality, it has become possible to pass Fortran-defined structured data type to C++ functions which receives class variables in the standard way. We use this functionality extensively to make FDPS callable from Fortran user programs. Roughly speaking, for Fortran particle data types, equivalent C++ class is generated according to directives (special comments) in Fortran source, and all necessary functions are automatically generated in FDPS side, and Fortran interface are defined.

We have released this version of FDPS on December 2016, and apparently quite a few users are now using Fortran interface.

10.3.3 Improvements on Particle-based CFD

SPH (Smoothed Particle Hydrodynamics) has been used in many field, including astrophysics, mechanical engineering and civil engineering. Recently, however, it was pointed out that the standard formulation of SPH has numerical difficulty at the contact discontinuity. The reason is that the formulation of the standard SPH requires that the density is differentiable, which is by definition no the case at the contact discontinuity.

We have been working on the possible solution on this problem. One approach is to reformulate SPH so that it does not use the density in the right-hand side of the equation of motion. We one way to achieve the density independence. We constructed an SPH scheme which uses artificial density-like quantity as the base of the volume estimator. It evolves through usual continuity equation, but with additional diffusion term. Thus, we can guarantee the continuity and differentiability of this quantity, except at the initial condition or at the moment when two fluid elements contact with each other. This scheme seems to work extremely well, and we are currently working on the way to extend this scheme so that it can handle free surface accurately.

We are also working on a completely different approach, in which we replace the SPH formulation to evaluate the gradient to other schemes. SPH has a known problem that its kernel estimate contains O(1) error, since the summation of contributions from neighbor particles is not guaranteed to be unity. The reason why SPH uses this mathematically inconsistent formulation is to achieve symmetry and conservation. In SPH discretization, interaction between two particles is symmetric, which guarantees the conservation of linear and angular momenta. However, the use of SPH approximation resulted in rather low accuracy, which limits the reliability of the results obtained using SPH. We have developed a completely different scheme, which can achieve much higher accuracy, while losing some of the nice features of SPH such as the symmetry of interaction.

Our new approach, which we call CPHSF (Consistent Particle Hydrodynamics in Strong Form), is based on high-order MLS (moving least square fit). In SPH, particles have mass and energy (or entropy). Particle mass is automatically conserved, and SPH differentiation is constructed so that the total energy is conserved. Thus, SPH is quite robust, since conserved quantities are always conserved. However, this formulation makes it practically impossible to construct high-order schemes, express boundary condition explicitly or handle contact discontinuity. Therefore, in CPHSF, we gave up the exact conservation of mass and energy, but instead achieved the conservation by the scheme which is of higher order in both space and time.

With this scheme, we can express both first- and second-type boundary conditions. However, with the current formulation, in order to use the second-type boundary conditions, we need to solve implicit equations for boundary particles, which effectively make the scheme implicit, even when explicit scheme is used for time

integration. We are currently working on possible ways to handle second-type boundary conditions with explicit time integration.

10.4 Schedule and Future Plan

We plan to improve the performance of FDPS further in FY 2017. In particular, we plan to improve the performance of user code for very large number of processes and also for short-range interactions.

10.5 Publications

10.5.1 Journal Articles

[1] Masaki Iwasawa ,Ataru Tanikawa, Natsuki Hosono, Keigo Nitadori, Takayuki Muranushi, Jun Makino, Implementation and performance of FDPS: a framework for developing parallel particle simulation codes, Publications of the Astronomical Society of Japan, Volume 68, Issue 4, id.54, 08/2016.
[2] Hosono, Natsuki, Saitoh, Takayuki R.; Makino, Junichiro; Genda, Hidenori; Ida, Shigeru, The giant impact simulations with density independent smoothed particle hydrodynamics, Icarus, Volume 271, p. 131-157, 06/2016.
[3] Hosono, Natsuki, Saitoh, Takayuki R.; Makino, Junichiro, A Comparison of SPH Artificial Viscosities and Their Impact on the Keplerian Disk, The Astrophysical Journal Supplement Series, Volume 224, Issue 2, article id. 32, 06/2016.
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[5] Rieder Steven, ,Kenworthy Matthew A., Constraints on the size and dynamics of the J1407b ring system, Astronomy & Astrophysics, Volume 596, id.A9, 5 pp, 11/2016.
[6] Natsuki Hosono, Masaki Iwasawa, Ataru Tanikawa, Keigo Nitadori, Takayuki Muranushi, Jun Makino, Unconvergence of Very Large Scale GI Simulations, Publications of the Astronomical Society of Japan, 2016/12/21
[7] Satoko Yamamoto, Jun Makino, A formulation of consistent particle hydrodynamics in strong form PASJ 2017/01/19
[8] Tomonari Sumi, Yutaka Maruyama, Ayori Mitsutake, and Kenichiro Koga, A reference-modified density functional theory: An application to solvation free-energy calculations for a Lennard-Jones solution, The Journal of Chemical Physics, Volume 144, Issue 22, P 224104, 14 June 2016.

10.5.2 Conference Papers

[9] Naoki Yoshifuji, Ryo Sakamoto, Keigo Nitadori, & Jun Makino, Implementation and evaluation of data-compression algorithms for irregular-grid iterative methods on the PEZY-SC processor, 2016 6th Workshop on Irregular Applications: Architecture and Algorithms (IA3), 58-61, Nov. 13, 2016.
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[11] Takayuki Muranushi, Seiya Nishizawa, Hirofumi Tomita, Keigo Nitadori, Masaki Iwasawa, Yutaka Maruyama, Hisashi Yashiro, Yoshifumi Nakamura, Hideyuki Hotta, Junichiro Makino, Natsuki Hosono, Hikaru Inoue, Automatic generation of efficient codes from mathematical descriptions of stencil computation, FHPC 2016 Proceedings of the 5th International Workshop on Functional High-Performance Computing Pages 17-22 22 September 2016

Chapter 11

Computational Climate Science Research Team

11.1 Members

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Yoshiyuki Kajikawa (Senior Scientist)

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Shoko Kojima (Research Assistant)

11.2 Research Activities

Our research team conducts the pioneering research work to lead the future climate simulation. In order to enhance the reliability of climate model, we have aimed to construct a new climate model based on the further theoretically physical principles. Conducting such a new model needs tremendously large computer resources. Therefore, it is necessary to design the model to pull out the capability of computers as much as possible. Recent development of supercomputers has a remarkable progress. Hence another numerical technique should

be needed under the collaboration of hardware research and software engineering for the effective use on the future HPC, including the K computer and Post K computer.

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

We have proposed the subject "Estimation of different results by many numerical techniques and their combination" as a synergetic research to MEXT from 2011. We develop a new library for numerical simulation. In this fiscal year, we improved computational performance of SCALE library and validation of its physical performance, aiming at the reliability of SCALE. In addition, for the user expansion and promotion, we vigorously maintained the user's manual and model document and held hands-on seminar twice. New developments are highlighted as follows.

11.2.1 Improvement of dynamical core in SCALE-RM

In atmosphere simulation, the calculation of the dynamical process that is a fluid dynamics calculation part is very important from the both sides of physical and computational performances. So far, it has been necessary to set the time step as the half of CFL based on the acoustic wave and numerical noise has appeared when the wind velocity was fast. We improved the numerical scheme of the dynamics process.

Because the most suitable schemes depend on the purpose of simulations, we made arbitrary combination of the time integration method and spatial difference schemes be chosen by a user (see the user's guide in https://scale.aics.riken.jp/). By using this framework, the combination of schemes suitable for real atmosphere simulation is examined. As a result, in comparison with the experiment by the conventional scheme, we achieved double speedup in the calculation of the dynamical part. From the viewpoint of physical performance, we confirmed that numerical noise was suppressed. This improvement also led to the prediction score in the forecast experiment.

11.2.2 Implementation of MPI-IO

From the viewpoint of I/O performance, it is recommended that files are accessed every process using rank IO function in the K Computer. On the other hand, from the viewpoint of programing for file management and pre- and post-processing, it is desirable to be a single file. This function has also an advantage that calculation nodes can be set flexibly at restarting the simulation. We implemented the file input and output function using MPI-IO, considering the user convenience with I/O performance. For this purpose, we used pnetCDF (http://cucis.ece.northwestern.edu/projects/PnetCDF/), coexisting netCDF (default format in SCALE-RM), using asynchronous I/O to gain the computational performance.

11.2.3 Validation of physical performance on SCALE-GM

To validate the physical performance of icosahedral dynamical core, NICAM-DC (prototype of SCALE-GM), our group participated the 2016 DCMIP (Dynamical Core Model Intercomparison Project: https://www.earthsystemcog.org/projects/dcmip-2016/). Through this activity, the ideal experiment cases of SCALE-GM were expanded.

11.3 Research Results and Achievements

Several outstanding research achievements highlighted as the following.

11.3.1 Disaster prevention research in establishment of COE project

Five subjects have been accepted since 2012 as the Hyogo-Kobe COE establishment project. One of subjects is "the computational research of disaster prevention in the Kansai area". In this subject, our team is responsible for the sub-subject of "Examination of heavy-rainfall event and construction of hazard map."

After the tuning of precipitation properties in the regional climate model used (SCALE-RM), we completed to perform 25-years downscaling simulations for present and future climate using climate data projected by MRI-AGCM3.2S as boundary conditions. The extreme precipitation, which is defined by the 25-year average of

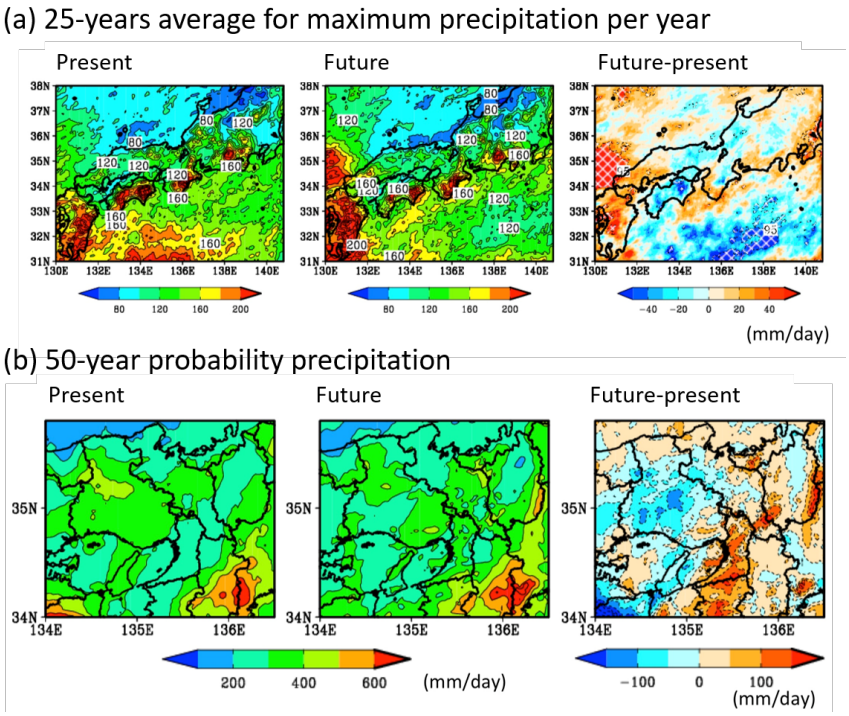

Figure 11.1: The result of COE project: (a)the 25-year average of maximum daily precipitation between June and September. (b) 50-year probability precipitation in this area

maximum daily precipitation between June and September, in present climate shows large value in the Kyusyu island and the Pacific side of Japan (Fig.11.1 (a)). The extreme precipitation in future climate is projected to be intensified over whole areas of Kyusyu island, while it is projected to be weaken over the Shikoku and Kansai regions. As a hazard map for heavy rainfall, we estimated a 50-year probability precipitation, i.e., daily precipitation with a probability of occurring one time during fifty years. The result shows that a 50-year probability precipitation is intensified in Osaka and the north part of Wakayama prefectures, whereas it is weakened in Hyogo prefecture except for some areas (Fig.11.1 (b)).

The above results were based on one climate projection estimated by single general circulation model (GCM). To improve the reliability of results, ensemble simulations using multiple climate projections by multi-GCMs are required in future. It is also important to understand a physical mechanism causing the regional climate change for evaluating the reliability: a new method is necessary to be established.

11.3.2 Statistics of dust devils in Mars

Dust devils in the Mars is one of most important phenomena in the Mars. We investigated the statistics of dust devil using SCALE-RM. For reliable result, the Large Eddy Simulation is adopted as the turbulence scheme with 5m grid spacing both in the horizontal and vertical directions (Fig.11.2). In a wide domain size of 20km x 20km, we could detect over 3000 dust devils, of which radius spread from several m to several hundred m (Nishizawa et al. 2016). Not only the statistics of horizontal radius but also of maximum wind speed and pressure drop were also investigated. The obtained information will provide useful information to manned exploration on the Mar and contribute to the Mars weather forecast.

11.3.3 High resolution simulation of nowthward black carbon transfer

We performed the aerosol transfer simulation, using the global model NICAM. The results indicated the high resolution with non-hydrostatic dynamics transferred the black carbon to Arctic region with quantitative agreement to observation. As shown in Fig 11.3, in the coarse resolution run, contrast between cloud and cloud-free area were not clear and wet deposition occurred over wide area. This led to too much wet deposition over wide area. On the other hand, the clear contrast appeared in the fine resolution run. As a result, appropriate amount of black carbon was transferred northward. Thus, the error is drastically reduced by the expression of detailed

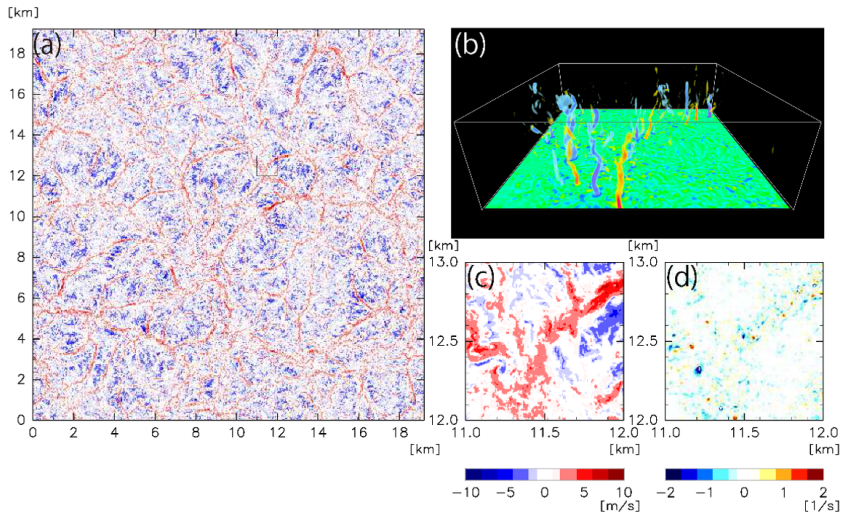

Figure 11.2: Large Eddy Simulation of dust devils in Mars

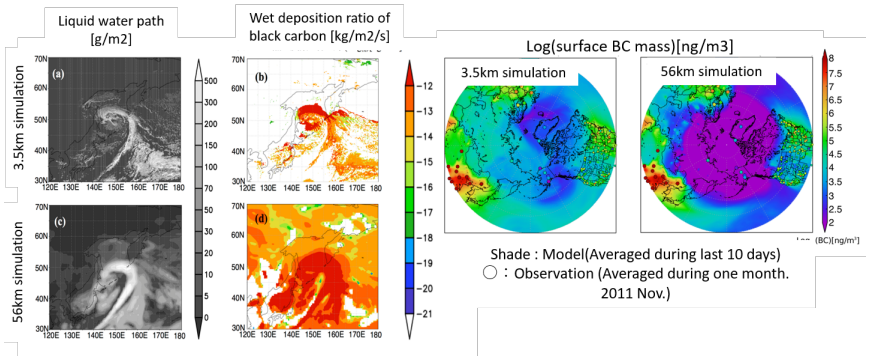

Figure 11.3: The result of high resolution simulation of black carbon transfer

structure of low and frontal system in high resolution. This mechanism in the mid-latitude directly improves to the sedimentation of black carbon in the polar region (right panel of Fig.11.3). This simulation suggests that global scale modeling with fine grid resolution is required for accurate representation of aerosol in Arctic and in Antarctic, otherwise, the ice-albedo feedback is underestimated.

11.4 Schedule and Future Plan

We continue to sophisticate the basic library SCALE. At the present, the main processes, both of dynamics and physics, have already been developed comprehensively. We will pursue higher usability for the outside users. We keep elaborating the advanced climate model based on schemes in principle and indicate a direction to future climate model. At the same time, not only to make computational and physical performance of simulation code higher but also to provide useful analysis methods of simulation results is a main issue in the next phase. This is of great importance for acceleration of scientific output and social outcome.

The research for contribution of prevention from future heavy rainfall event and thermal environment in urban is also continuous in the second term COE project, which starts from the FY2017. There are still many uncertainties for the future prediction due to model bias. One of main causes is bias in regional model itself. Since SCALE has already implemented many components and schemes, construction of different models is easy. This advantage would be able to evaluate biases caused from regional models. This is done by the way of multi-model ensembles with data assimilation science.

11.5 Publications

11.5.1 Journal Articles

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Chapter 12

Complex Phenomena Unified Simulation Research Team

12.1 Members

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12.2 Research Activities

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

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

computer costs and communications among processor cores. Different mesh topology and hence data structures among each simulation and treatment of different time or spatial scales also deteriorate single processor performance. We understand that one of the keys to solve these problems is to adopt unified structured mesh and data structure among multiple simulations for coupled phenomena. As a candidate of unified data structure for complicated and coupled phenomena, we focused on the building-cube method (BCM) proposed by Nakahashi[1].

12.3 Research Results and Achievements

12.3.1 Development and validation of Euler based structured analysis method

Currently, in the numerical analysis of structures with complicated shapes such as automobiles, the Lagrangian finite element method using a unstructured mesh is the de facto standard. The Lagrange type finite element method using an unstructured mesh has the following problems. First, it is difficult to improve parallelization efficiency compared with orthogonal meshes. Secondly, in many cases, it takes a lot of time and know-how to generate a complicated mesh. Thirdly, it is complicated to couple with mesh and different numerical analysis of description method as in fluid analysis. Based on the above background, this study is developing Euler type dynamic structural analysis based on BCM. In BCM, since fine cube can be arranged locally, it is easy to capture the solid interface and it is easy to improve parallelization efficiency. Also, since it is a spatially fixed orthogonal mesh method, coupling with fluid analysis is easy, and there is an advantage that a mesh can be easily generated even in a complex shape. In FY2016, Euler type dynamic structural analysis was implemented in the analysis code CUBE and basic verification was carried out. Using equations of motion that are unified with solid and fluid under the assumption of incompressibility as the basic equation. Second-order Adams-Bash force method is used for time integration, and a finite volume method based on a coherent lattice with a simple data structure is used for space discretization. The solid interface is captured by the VOF method and the advection equation of the VOF function is calculated by the WENO method of fifth order accuracy. Neo-hook body as a constitutive law of solid, Newtonian fluid is assumed as a constitutive law of fluid. In the Euler type structure analysis, it was difficult to impose the load boundary condition on the interface because the nodes of the space-fixed mesh do not follow the solid interface, but in this study, Continuous surface stress (CSS) model[2], we have developed a method to assign load boundary conditions.

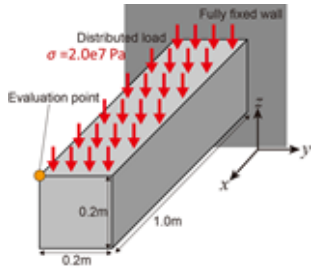


Figure 12.1: Three-dimensional cantilever beam

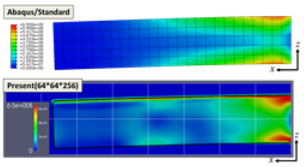


Figure 12.2: Mises stress distribution

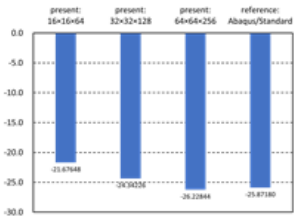


Figure 12.3: Displacement of evaluation point

This method was verified by the bending problem of three dimensional cantilever shown in Fig.12.1. The reference solution is the result by Abaqus / Standard. Fig.12.2 shows the Mises stress distribution at 1 ms, and Fig.12.3 shows the displacement of the evaluation point (Fig.12.1) at 1 ms. From Fig.12.2, it can be confirmed that the Mises stress distribution is roughly in agreement, and it can be confirmed that the displacement of the evaluation point shows quantitatively good agreement when the cell division number is 64 ?64 ?256.

12.3.2 Improvement of accuracy of automobile aerodynamics analysis by full vehicle model and calculation speeding up

12.3.2.1 Reduction of calculation load by introducing local mesh refinement near wall surface

In the BCM, the calculation grid in the vicinity of the wall is subdivided until it reaches the user-specified maximum division number from the intersection judgment of the input CAD data and the Cartesian grid.

Therefore, in the vicinity of the wall surface, the resolution is always the same regardless of the location, but if it is possible to locally adjust the resolution of the resolution according to the characteristics of the flow field, it is efficient. In order to perform this local subdivision, we developed an improved of the framework so that individual numbers can be assigned to each part of CAD data, and the number of refinement can be specified for each number. Granting of numbers can be easily performed by GUI operation in both general CAD software and grid generation software, and this is a method that does not impair user convenience. Fig.12.4 shows a diagram of the CAD data used in this calculation. Indicates that each color has a different part number. The example of the computational grid obtained is shown in Fig.12.5. The total number of grid is about six times less than the number of grid when using a single resolution overall. This means that the calculation load can be saved six times for the same resolution calculation. It is confirmed that aerodynamic analysis is performed using this calculation grid and analysis is possible with the same calculation error as before.

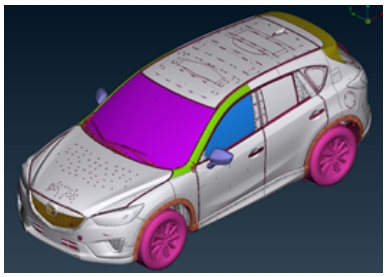


Figure 12.4: Example of CAD data with part ID

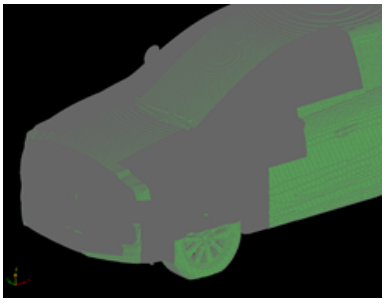


Figure 12.5: Examples of calculation grid using local refinement

12.3.2.2 Improvement of accuracy of aerodynamic analysis by full vehicle model

We improved the analysis accuracy of aerodynamic analysis for the following actual vehicle models provided by domestic automobile manufacturers. This was obtained by fitting with algorithm change of the incompressed flow analysis framework, tuning of the fluid force calculation method, and actual measurement by detailed examination of the automobile model shape. The Table.12.1, We compare the difference of aerodynamic drag coefficient (Cd) by two aerodynamic specification models using realistic full vehicle model with the numerical values obtained by wind tunnel measurement. The absolute value of Cd is estimated to be 7 to 8% erro for small-car, and for SUV and hatchbacks with 1 to 2% error. And here the absolute value is not so meaningful, but the difference of 2 specification is important. It is practically important to precisely predict delta Cd (任 d).

Table 12.1: Analysis result of drag coefficient difference (任 d) for two aerodynamic specifications

Model	Exp.	FY2015	FY2016
Small-car	-0.030	-0.061	-0.026
SUV	+0.004	+0.006	+0.003
Hatchback	+0.045	-0.005	+0.024

Incidentally, since the above-described part contains confidential information, the image and the absolute value for which the vehicle type is specified are omitted here.

12.3.3 The CAA (Computational Aeroacoustics) of full-scale road vehicle by CUBE

The fluid-induced acoustics field around vehicle is investigated. The all-speed compressible flow solver is adopted for solving the flow field and acoustics data. The local refinement mesh technique is used as Fig.12.6 to enhance the mesh resolution in the flow field where strong interaction between fluids and vehicle may occur.

The iso-surface of instantaneous Q-criterion near vehicle is shown in Fig.12.7. The color of iso-surface indicates the magnitude of velocity. There are two regions, which near A-pillar and downstream of the side mirror, with highly developed vortex structures might generated most of the acoustics sources. Shown in

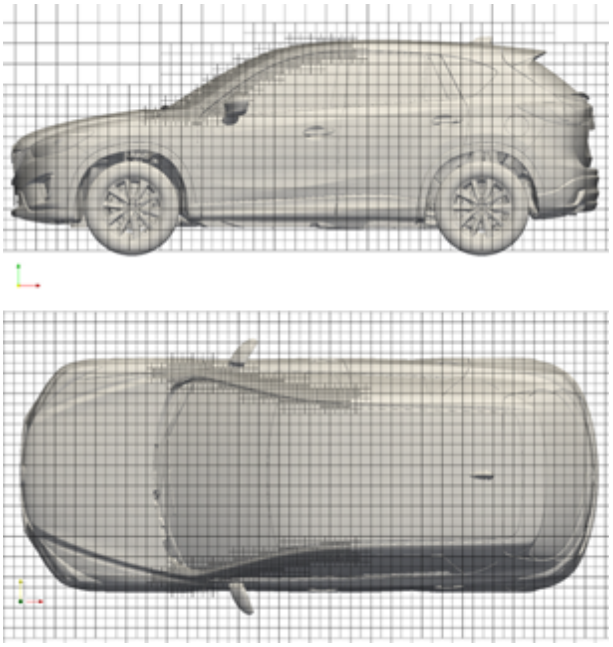


Figure 12.6: Mesh distribution around vehicle

Fig.12.8, these kind of features can be also identified by the streamlines near A-pillar and the close view of the side mirror.

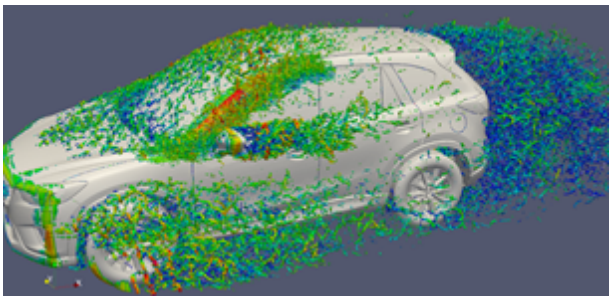


Figure 12.7: The iso-surface of instantaneous Q-criterion

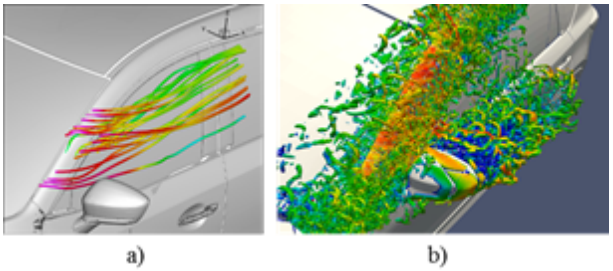


Figure 12.8: Close view of (a) streamlines and (b) Q-criterion

The experimental data, which provided by automobile company for validation are beam-forming contour plots of side window as shown in Fig.12.9(a) and Fig.12.10(a). In order to distinguish the aeroacoustics sources, the time-dependent pressure data are transform to frequency field by Fast Fourier Transform (FFT) near side window region. Shown in Fig.12.9(b) (h) and Fig.12.10(b) (h), the iso-surface in different power level of acoustics are compared with experimental data of both low and high frequencies.

The qualitative agreement of CUBE with beam-forming acoustics contour plot shows that the CAA data

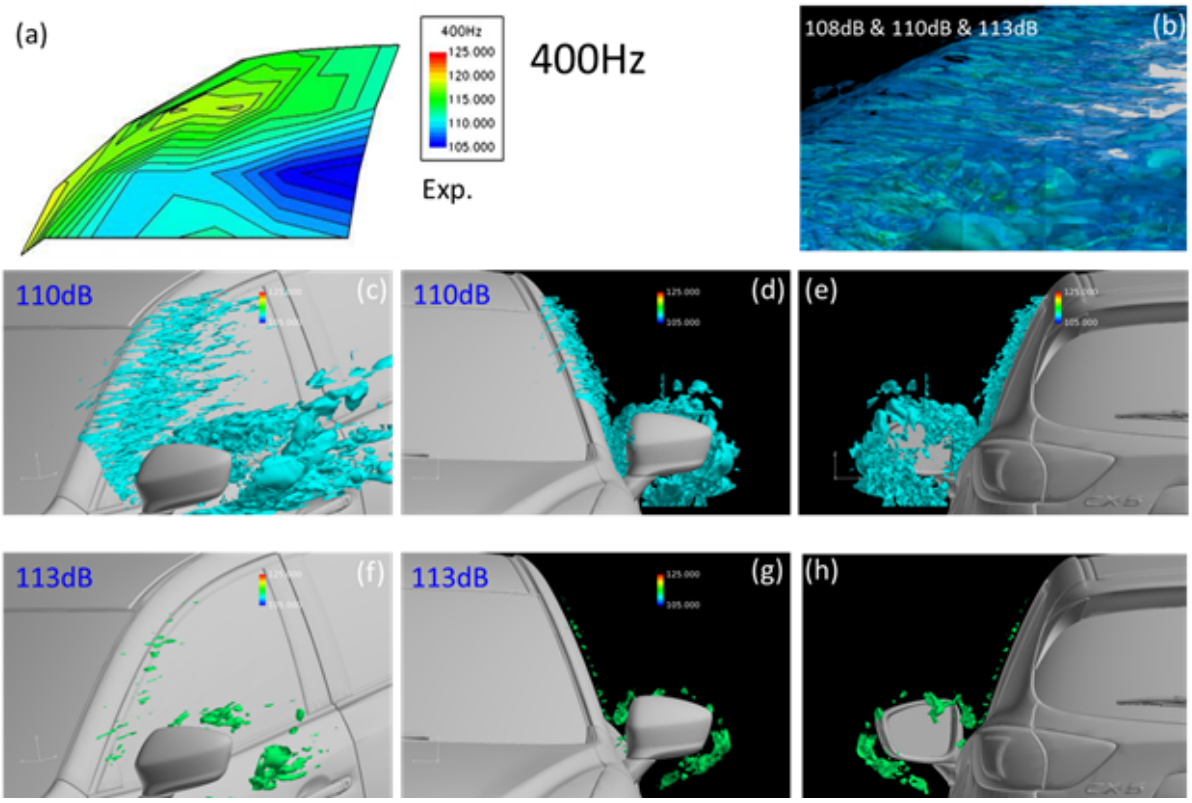


Figure 12.9: Acoustics power level of (a) experimental and (b) (h) numerical results of 400Hz

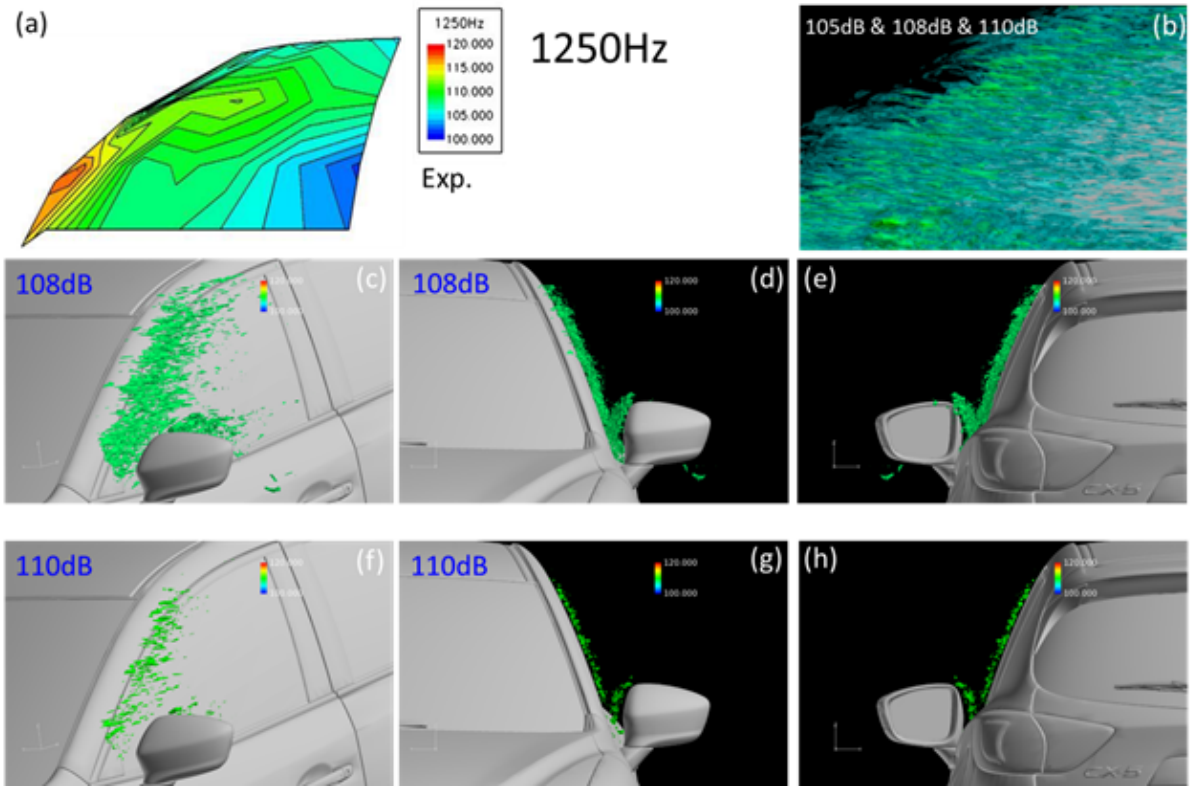


Figure 12.10: Acoustics power level of (a) experimental and (b) (h) numerical results of 1250Hz

could be a reference for the usage of aero-acoustics design of vehicle industrial applications.

12.3.4 Development of automobile engine combustion simulation technology

In order to realize automobile engine simulation, we developed a combustion analysis method that reproduces the valve and piston motion based on the fluid-structural unified analysis framework.

12.3.4.1 Chemical reaction model

The chemical reaction framework is added into the in-house CFD code CUBE by equilibrium model with G-equation interface tracking method for multi-species and combustion calculation. Fig.12.11 shows the flow chart of the whole framework. Compressible flow solver and chemical reaction solver are communicated with each other every numerical time step to update the flow field information such as mole fraction of species, temperature, pressure, density, heat capacities and so on.

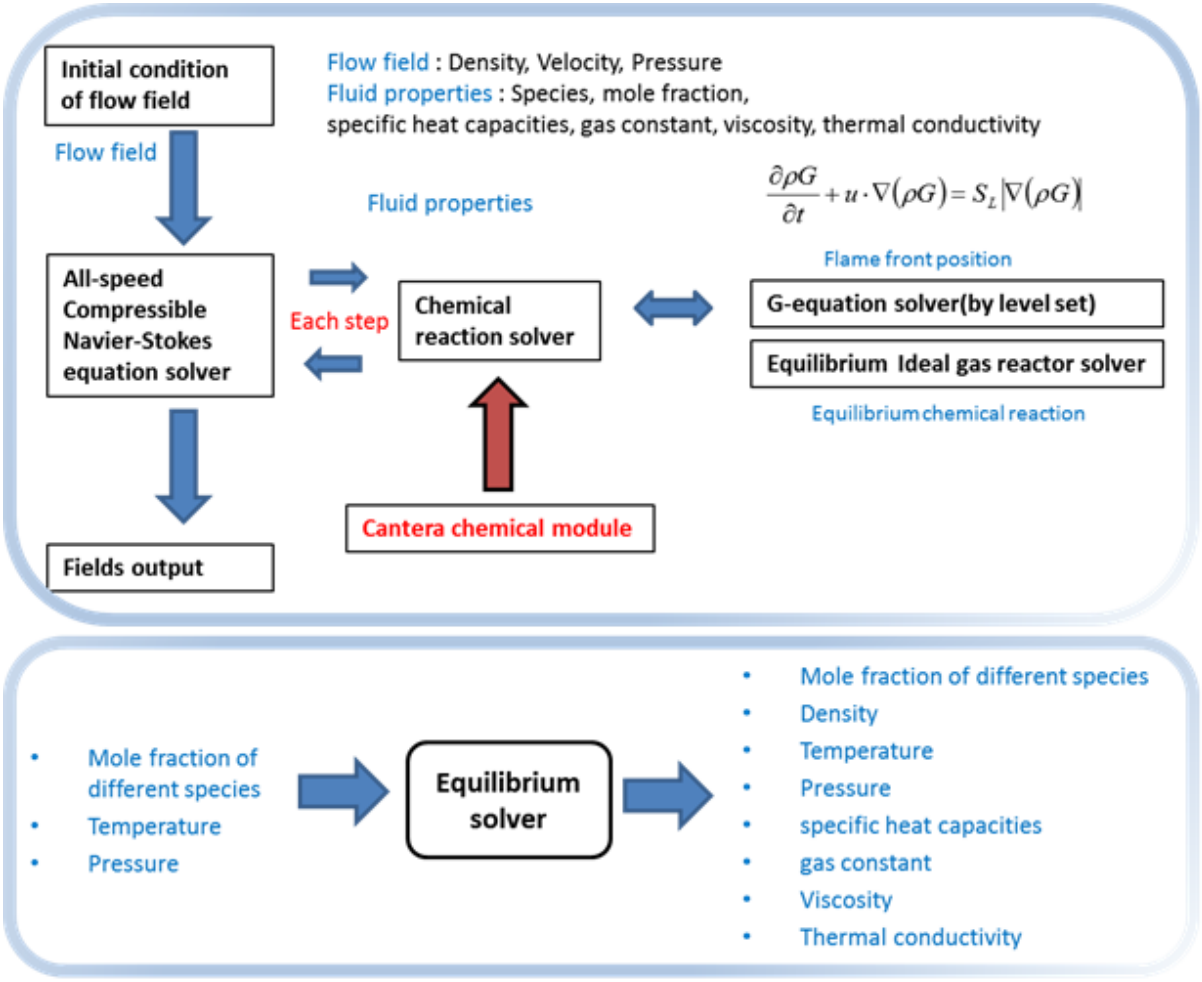


Figure 12.11: Chemical reaction framework of CUBE

A piston geometry is used for the qualitative validation for the chemical reaction framework as Fig.12.12. The piston plate moves periodically and fluids inside the chamber is compressed and ignited. Fig.12.13 shows the averaged pressure variation near the top end region with time in one cycle. Before the ignition point the pressure is increased due to the compression process, and then ignition started with the chemical reaction, which makes the pressure continuously raised. When it goes to the expansion process with all the fluids burned, the pressure finally decreased but still higher than the initial pressure, which shows a reasonable result.

In conclusion, the chemical reaction of CUBE makes it more useful for the industrial applications such as engine combustion simulation and other aerothermodynamics problems, and more quantitative validation and multi-species with spray modeling is needed for the future use.

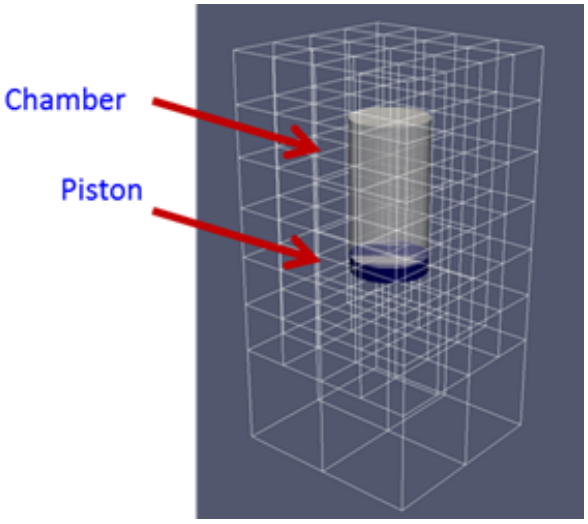


Figure 12.12: Piston model

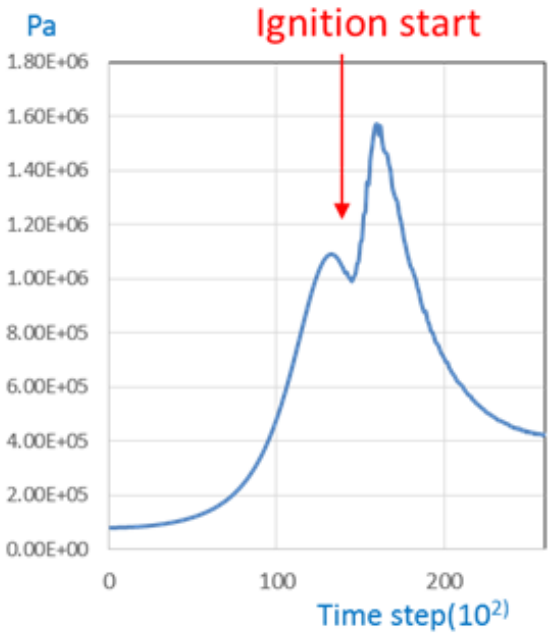


Figure 12.13: Averaged pressure variation near the top end with time

12.3.4.2 Fuel Spray Modeling

Fuel spray atomization in one of the integral aspects of internal combustion engines. The level of fuel atomization determines how well the thermal energy of the fuel is utilized in combustion process, thus atomization is closely linked to the thermal efficiency of the engine. Therefore, numerical modeling of internal combustion engines necessitates fuel spray modeling.

In a typical fuel spray the atomization leads to droplets as small as few m and as large as few millimeter. Numerical simulations that fully resolves the droplets at all the scales are not feasible by today 寰洒 HPC facilities as the mesh resolution necessary to resolve the smallest drops is prohibitively small. In this scenario, reduced order models for modeling spray atomization are invaluable.

The reduced order model we consider can be characterized as follows:

- The atomized spray droplets are modeled as discrete set of Lagrangian particles.
- A set of characteristics are associated with each droplet.

- The velocity and position are modeled via drag model.

$$\frac{\partial \mathbf{x}}{\partial t} = \mathbf{v} \qquad \frac{\partial \mathbf{v}}{\partial t} = \mathbf{F}_d + \mathbf{g}, \tag{12.1}$$

- The temperature and radius are modeled by evaporation model

$$\alpha_T \dot{T} + \beta_T T = \gamma_T, \tag{12.2}$$

$$\frac{\partial r}{\partial t} = \frac{(\rho D)_{air}}{\rho_d r} B_d Sh_d. \tag{12.3}$$

- Finally, the shape of the droplet are modeled by a breakup model

$$\ddot{y} + \alpha \dot{y} + \beta y = \gamma. \tag{12.4}$$

As the fuel spray droplets are modeled as discrete set of Lagrangian particles, incorporation of spray model into CUBE was straight forward through the building cube Lagrangian data structure. The implementation was validated through the simulation of p-xylene fuel spray and comparing with experimental data. The result of the simulation is shown in Fig.12.14 below. In Fig.12.15. temporal evolution of spray droplets from a test simulation of n-heptane spray is show. The simulation parameters of this simulation is detailed in Table 12.2.

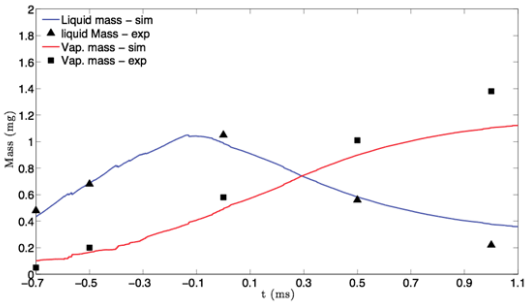


Figure 12.14: Comparison vapor penetration and vapor mass of p-xylene spray as a function of time

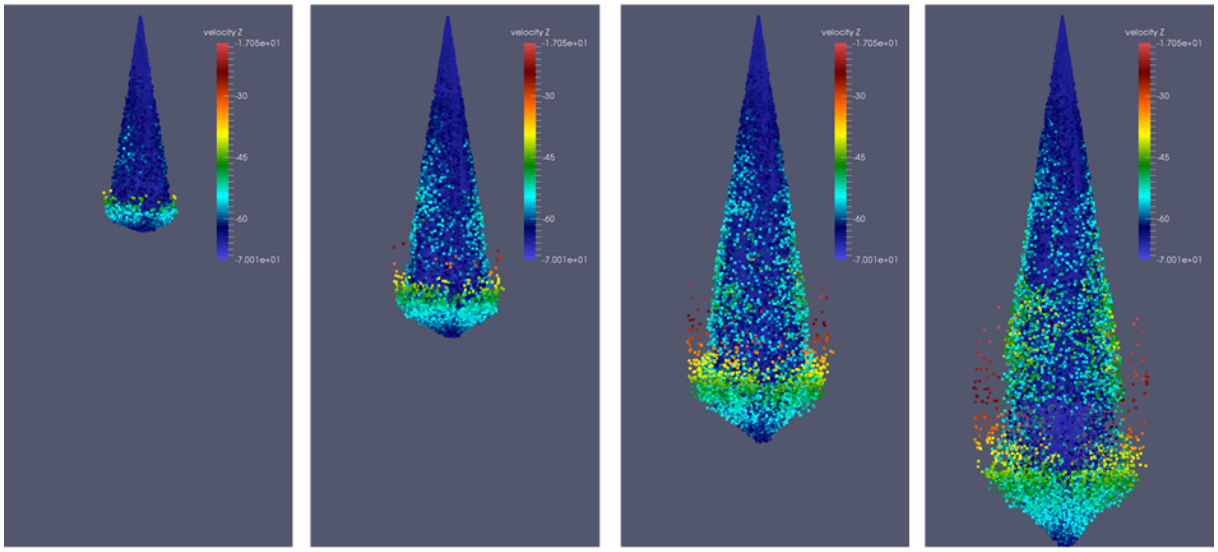


Figure 12.15: Evolution of spray droplet particles

Table 12.2: Simulation Parameters of test spray simulation

Mesh	1Million
dx	0.007m
Fuel	N-heptane
Nozzle cone-angle	20deg
Injection Velocity	60 m/s
No. Particles	50000
Droplet redius	4e-4 to 4e-6m

12.3.5 Unsteady aerodynamic analysis of automobiles in turning maneuvers

The aerodynamic performance and stability a vehicle is strongly influenced by the crosswinds during cruise and by lateral flow during turning maneuvers. Ideally, it is desirable simulate such real world driving conditions in wind tunnel experiments. But, it is difficult to reproduce real world driving conditions during wind tunnel experiments due to the nature of force measurement techniques employed and the fact that only a unidirectional winds can be generated in a wind tunnel. Force measuring transducers are typically placed at the base of the wheels of the vehicle. This implies that wheels can neither be rotated nor steered during experimentation. Furthermore, visualization of three dimensional flow field around the vehicle, although possible in principle, is very expensive and difficult to achieve in experiments. Thus, we resort to numerical techniques that can enable us to emulate real world driving conditions in numerical simulations that can enable accurate measurement of flow field and visualization of the flow.

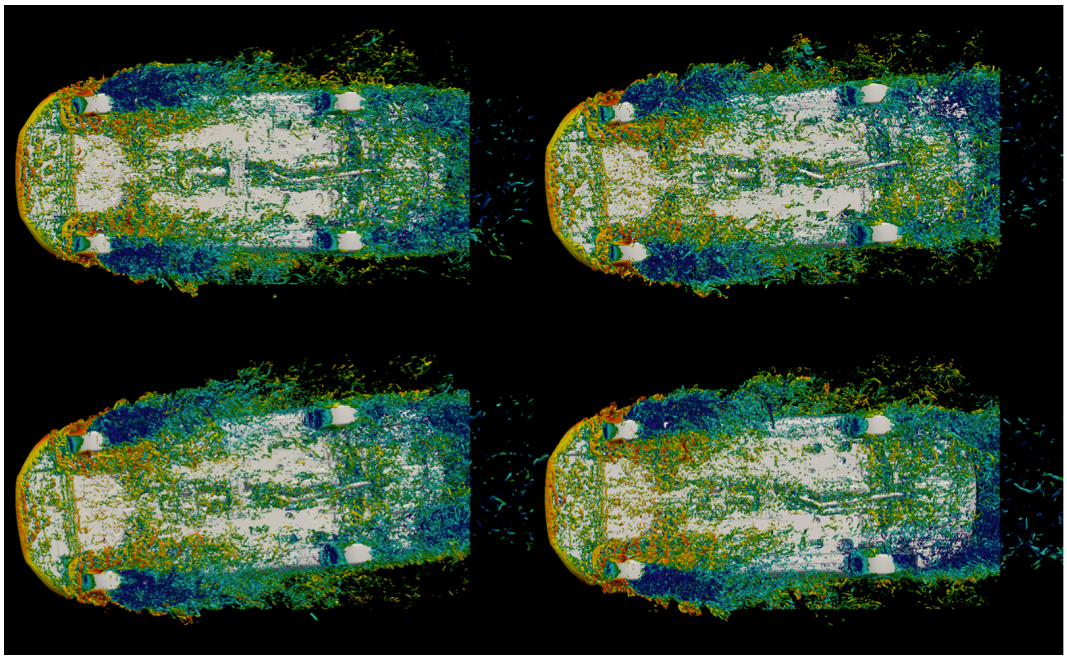


Figure 12.16: Visualization of flow around vehicle during lane change maneuver through q-criterion. The sequence of images show the vehicle in lane change maneuver.

The goal of this work is to investigate the flow physics encountered around a vehicle during the lane change maneuver. The mesh used for the simulation and the velocity profile of vehicle during lane change maneuver are shown in the figure above. The equations of motion of the system are described below. The velocity of the vehicle including its linear and rotational component of the motion is given by

$$\mathbf{u}_{turn} = [u_l, v_l, w_{l]}] + [\omega_x, \omega_y, \omega_z][r_x, r_y, r_z]^T \tag{12.5}$$

The motion of the vehicle is split into two components namely, linear and rotational (as is shown in the equation above). The linear component of the vehicle are imposed as boundary condition to the computational domain; the rotational component of the motion is imposed through the immersed boundary method. As

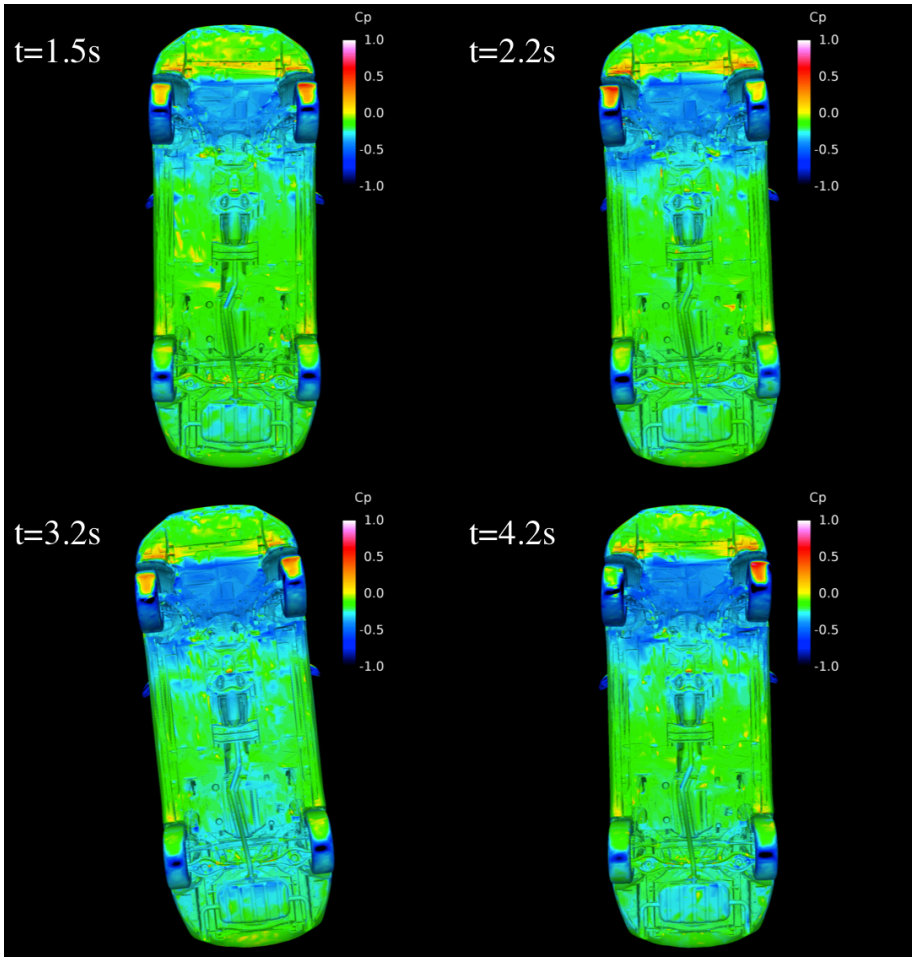


Figure 12.17: Coefficient of pressure projected on the surface of the vehicle.

the linear velocity of the vehicle is unsteady, merely imposing it as boundary condition will not suffice. The acceleration due to the lane change maneuver has to accounted in the momentum equation as shown below.

$$\frac{D\mathbf{u}}{Dt} = -\frac{1}{\rho}\nabla p + \frac{\mu}{\rho}\nabla^2\mathbf{u} + \mathbf{f}_{turn}, \text{ where } \mathbf{f}_{turn} = \frac{\partial}{\partial t}[u_l, v_l, w_l]$$

The corresponding boundary conditions on the computational domain boundaries are:

1. X^-: $\mathbf{u}_{in} = [u_l, v_l, w_l]$, X^+: $\partial\mathbf{u}/\partial\mathbf{n} = 0$
2. Y^{+-}: $\mathbf{u}_{Y^{+-}} = [\partial u/\partial y, \partial v/\partial y, 0]$
3. Z^{+-}: Slip, no penetration

In the present simulations, Z component of the linear velocity of the vehicle is ignored, hence we use slip boundary condition in the Z direction. Lastly, the velocity condition for the immersed boundary method is imposed as follow.

$$\mathbf{u}_{ib} = [\omega_x, \omega_y, \omega_z][r_x, r_y, r_z]^T$$

In Fig. 12.16 & 12.18 visualizations of the iso surfaces of q-criterion and the coefficient of pressure projected on the surface of the vehicle are presented. While the more visualization of the flow field was carried out, for the purposes of the document, these two representative visualization will perhaps suffice. In the lane change maneuver, the vehicle is in linear motion from t=0 to t=2 s, the actual lane change maneuver begins at t=2s and continues until t∼4.2s and then the vehicle continues in a linear motion. During the maneuver, the lateral velocity first increases in magnitude from 0 to 3 m/s up to t∼3.1s, after which it decreases back down to 0. Here, time t∼3.1s is an inflection point in the lateral acceleration, i.e. the lateral acceleration changes sign. All

other components of the vehicles velocity exhibit similar during the period of the maneuver. The component of velocity that is of interest is the roll angle.

In Fig. 12.18a the roll angle is plotted as function of time. Similar to lateral acceleration, roll angle also has an inflection point around t∼3.2s. The force on the vehicle during the maneuver as plotted in Fig. 12.18b. The forces are oriented with the vehicles longitudinal axis as the vehicle turns. The trend of the forces after the start of the turning maneuver is predicable up to the inflection point (t∼3.2s). From t=2.2s, which is after the start of the turn, the lateral force deviates from its zero mean and exhibits negative values and monotonically increases in magnitude until the infection point (t∼3.2s). From t∼3.2s onwards, while the there is no change in behavior of the axial drag force, both lateral and lift forces exhibit interesting behavior. The lateral force which was increasing in magnitude begins to decrease and return back to the zero mean. The behavior of the lateral force is strongly correlated with the trend of the roll angle. From the beginning of the turn maneuver until the inflection point, the roll angle is positive, this implies a net negative force on the vehicle. After the inflection point the positive roll angle gradually changes to negative value before finally returning to zero, this implies that the net negative force on the vehicle has to reduce and tend towards a positive value as seen in Fig. 12.18b.

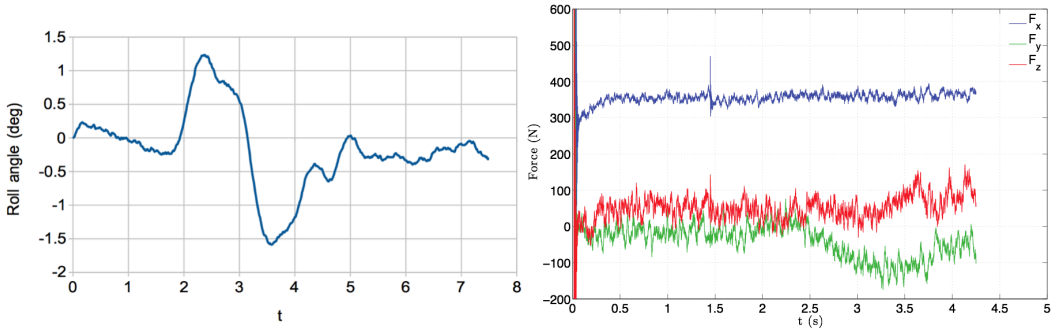


Figure 12.18: a) Roll angle plotted as a function of time. b) Forces oriented along the longitudinal axes of the vehicle as it undergoes the lane change maneuver.

Lastly, it is not clear as to what is the cause of the behavior of the lift forces. Until the inflection point the lift force has a relatively constant mean value. Beyond the inflection point the lift force suddenly start to increase in magnitude. While time at which lift force starts increasing is well correlated with the inflection point of the roll angle and the lateral acceleration, the root cause of this increase in lift force is not known. The increase in lift forces at the inflection point can also be observed through the pressure coefficient on the bottom surface of the vehicle in Fig. 12.16. Of the four time snapshots in Fig. 12.16 it is only at t=3.2s that we see a net greater quantity of dark blue color (or negative value of pressure coefficient). This implies that there is greater negative pressure at the bottom of the vehicle during the inflection point leading to an surge in the lift forces.

12.3.6 Real city block calculation related to wind HPC consortium

In order to analyze the boundary layer turbulence generated in urban canopy using incompressed unified solution method, we verified the accuracy of the Immersed Boundary Method for complex shape data, acquisition method of surface pressure data, designation method of inflow disturbance, spatial probe point data of interpolating method. This study aims to investigate the development process of the turbulent boundary layer using the topography data of the 25?2 km area in the central Tokyo area, and to investigate the influence on the development of the urban canopy boundary layer by the introduction of the inflow turbulence. An outline of the calculation region used is shown in Fig.12.19, and an example of the analysis result obtained is shown in Fig.12.20.

From the distribution of turbulence statistics, it is possible to investigate the urban surface roughness, the influence by the windward side building group, etc. However, since the calculation point does not exist on the wall boundary in Immersed Boundary Method, several evaluation methods are conceivable. So, we have verified the accuracy of methods using square cylinder model. Fig.12.21 shows the computational grids (Cubes) used in this study. Fig.12.22 shows the pressure distribution on the square cylinder surface obtained in this study. The solution of the CUBE uncompressed solution framework shows good results compared with the Immersed Boundary Method by the unstructured grid and other software, but the difference of measurement points used

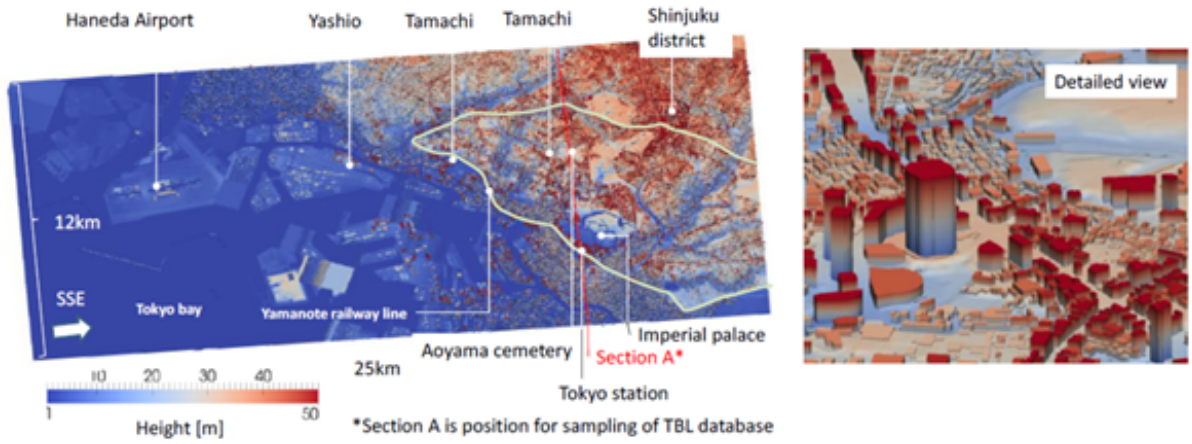


Figure 12.19: Outline of calculation area

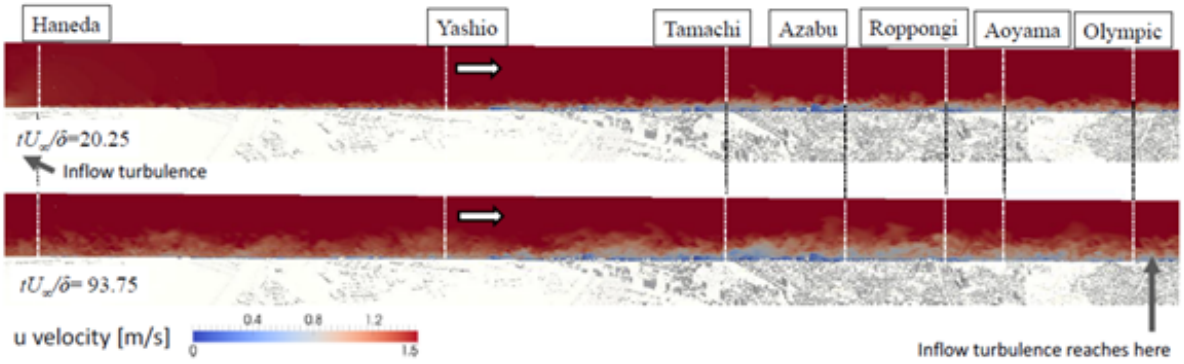


Figure 12.20: Effect of inflow turbulence condition on turbulent boundary layer development

for surface interpolation showed about several % error. Currently, weighting function for interpolation by distance is the most effective method, but problems such as failure to find an appropriate point for interpolation when we used complicated shapes, are left. So, further investigation is planned in the future.

12.4 Schedule and Future Plan

(1)Five-year objectives and goals toward 2017

- Construction and development of the simulation technology for bringing out the performance of K-computer
- Proposal of the technological trend of HPC simulation toward EXA-scale

(2)Long-term objectives

- Establishment of the research and development center for industrial simulation technology
- Contribution to computer science by expanding the developed simulation technology to different fields

(3)Time schedule

12.5 Publications

[1] Nakahashi, K., "Building-Cube Method for Flow Problems with Broadband Characteristic Length," Computational Fluid Dynamics 2002, Springer Berlin Heidelberg, 77–81, 2003.

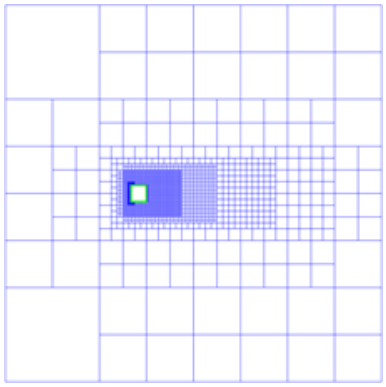


Figure 12.21: Calculation grid of square cylinder model

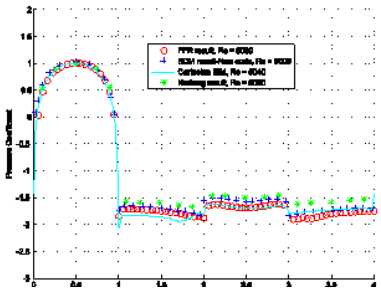
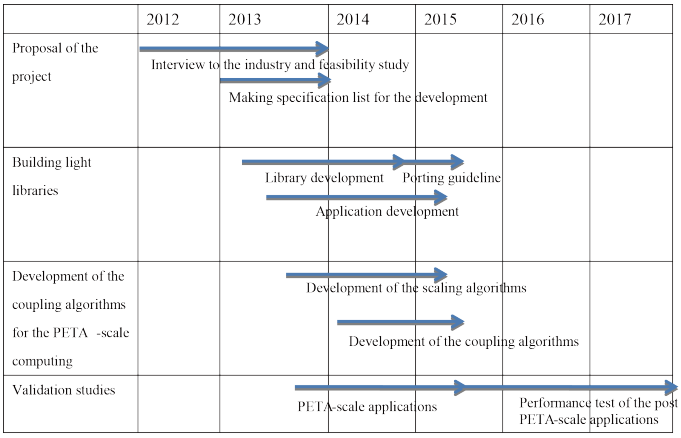


Figure 12.22: Surface pressure prediction accuracy verification by square cylinder model



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[7] Nishiguchi, K.,Okazawa, S., "Contact analysis using Eulerian XFEM",Proceedings of the conference on computational engineering and science, 21, 2016.

[8] Okawa, Y., Okazawa, S.,

Nishiguchi, K., "Eulerian solid-fluid interaction analysis",Proceedings of the conference on computational engineering and science, 21, 2016.

[9] K. Nishiguchi, S. Okazawa, "Fixed-mesh Eulerian Contact Formulation using X-FEM",Proceedings of 12th World Congress on Computational Mechanics,paper No.151379, 2016.

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[11] Tetsuro Tamura, Hidenori Kawai, Kazuaki Uchibori, Rahul Baled, Keiji Onishi, Makoto Tsubokura, Koji Kondo, Tsuyoshi Nozu, "High performance computation by BCM-LES on flow and pressure field around buildings", 8th International Colloquium on Bluff Body Aerodynamics and Applications,Boston, USA, 2016.

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[16] Tetsuro Tamura, Hidenori Kawai, Rahul Bale, Keiji Onishi, Makoto Tsubokura, "Application of BCM-LES model to flow and pressure fields over urban roughness", 69th Annual Meeting of the APS Division of Fluid Dynamics, 2016.

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[24] Kondo, K., Tamura, T., Kawai, H., Tsubokura, M., Onishi, K., Bale, R., "Influence of Small Topography on Average Wind Speed Distribution of Turbulent Boundary Layer Developed on Urban Area", Proceedings of annual meeting Architectural Institute of Japan, 2016.

Chapter 13

HPC Programming Framework Research Team

13.1 Members

Naoya Maruyama (Team Leader)

Motohiko Matsuda (Research Scientist)

Shinichiro Takizawa (Research Scientist)

Mohamed Wahib (Postdoctoral Researcher)

Keisuke Fukuda (Research Associate)

An Huynh (Student Trainee)

Satoshi Matsuoka (Senior Visiting Scientist)

Tomoko Nakashima (Assistant)

Aya Motohashi (Assistant)

13.2 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.

13.3 Research Results and Achievements

13.3.1 KMR

13.3.1.1 A Scalable Multi-Granular Data Model for Data Parallel Workflows

A wide range of scientific applications, including weather modeling, molecular dynamics and astrophysics, are run on large scale parallel computing systems. Obtaining scientific insights, however, requires executing those applications multiple times typically with different parameter configurations with different applications running concurrently, composing parallel workflows. Tasks in such a workflow typically run with multiple processes but the degree of parallelism often varies, resulting in the different numbers of tasks with the different numbers of processes. For example, a climate simulation with data assimilation can be realized by an ensemble execution

```
  # Create a DataStore
  # Initial Split: <N,8,8,8,8>
  # Dimensions
  #   1st      : ensembles
  #   2nd - 5th: simulation space (x,y,z,t)
1 ds0 = DataStore(4,64,64,64,64)
2 ds0.load_parallel(task_load)

  # Execute Dirac equation solver
3 ds0.set_split(<A,8,8,4,4>)
4 ds0.map(ds0, task_dirac, <A,N,N,N,N>)

  # Restore to the default layout
5 ds0.set_split(<N,8,8,8,8>)
6 ds0.map(NULL, task_restore, <N,N,N,N,N>)
```

Figure 13.1: BQCD pseudo-code that uses our model

of a climate model with different input values, followed by statistical adjustment of physical properties using real observation data. In the former phase, each task of the climate model is a parallel application with the whole simulation region split among parallel processes. In the latter phase, a statistical analysis on each grid point in the simulation region is run using all ensemble output and observation data of the point. Though a task in the former phase requires multiple processes, a task in the latter phase only requires a single process but the number of tasks is much larger. Moreover, processes in each phase have completely different data access patterns. Appropriate data decomposition and arrangement to processes are required between these two phases. Otherwise, performance degradation occurs due to unnecessary remote access.

To efficiently execute these applications, it is necessary to satisfy requirements for degree of parallelism, number of ensembles and data access pattern of all tasks that compose the applications. Application developers have to take the following three steps to write code that satisfies the above requirements for each task: (1) allocate enough number of processes to each ensemble, (2) decompose input data and arrange them to processes and (3) execute the task. Coding of these steps is highly troublesome and error-prone because data arrangement in (2) requires correct decomposition and transfer of the input by considering data access pattern. Moreover, as the implementation effort is in proportion to the number of tasks in a workflow, it becomes even worse for larger applications. Though the above problem is a common issue for applications irrespective of science fields, there are no common effective solutions and the reality is that developers have to hand-write the troublesome codes.

To solve the problem, we propose a multi-view data model that allows the user to create multi-dimensional arrays with adaptive granularities of decomposition to achieve efficient execution of data parallel workflows. Our framework conducts data arrangement and affinity-aware task scheduling as specified by the user with straightforward programming constructs (Fig. 13.1). We present a prototype implementation for distributed-memory parallel systems using MPI with APIs for C, C++, and Fortran. A case study using a lattice QCD code called BQCD, which is developed by Nakamura from AICS Kuramashi team, demonstrates that our framework can reduce the programming effort required to implement the application compared to a conventional MPI-based implementation with performance penalties up to 17% (Fig. 13.2 and Fig. 13.3).

13.3.2 High Level Framework for High Performance AMR

Adaptive Mesh Refinement methods reduce computational requirements of problems by increasing resolution for only areas of interest. However, in practice, efficient AMR implementations are difficult considering that the mesh hierarchy management must be optimized for the underlying hardware. Architecture complexity of GPUs can render efficient AMR to be particularity challenging in GPU-accelerated supercomputers. This work presents a compiler-based high-level framework that can automatically transform serial uniform mesh code annotated by the user into parallel adaptive mesh code optimized for GPU-accelerated supercomputers. Experimental results on three applications show that the speedups of code generated by our framework are comparable to hand-written AMR code, while achieving good and weak scaling up to 3,640 GPUs.

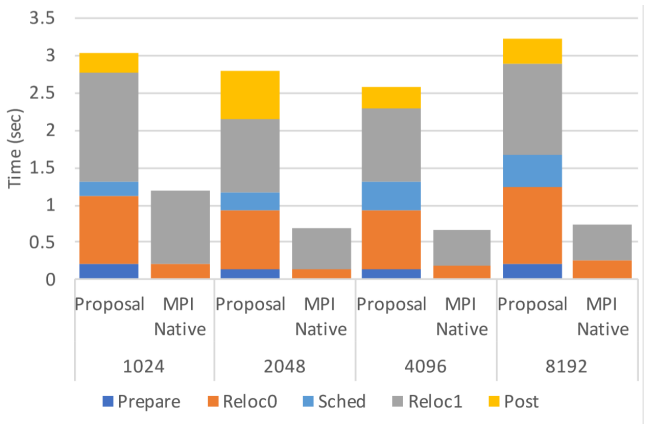

Figure 13.2: Comparison of overhead for data arrangement between our model and MPI Alltoall using BQCD: Strong Scalability

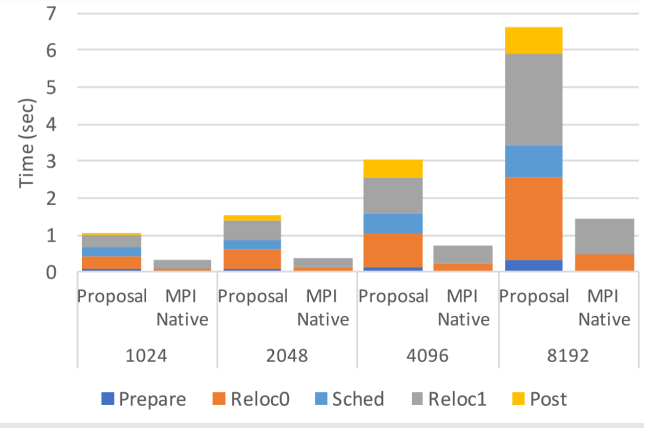

Figure 13.3: Comparison of overhead for data arrangement between our model and MPI Alltoall using BQCD: Weak Scalability

13.3.2.1 Introduction

In many scientific and engineering simulations, Partial Differential Equations (PDEs) are solved in a uniform mesh arrangement by using finite difference schemes, referred to as iterative stencils. Typically, the resolution of the mesh is uniformly set to the highest resolution to provide accurate solutions. For meshes that require only high resolution for some portions of the mesh, an alternative method, known as Adaptive Mesh Refinement (AMR), can be used instead of the uniform mesh. The AMR method solves the problem on a relatively coarse grid, and dynamically refines it in regions requiring higher resolution. However, AMR codes tend to be far more complicated than their uniform mesh counterparts due to the software infrastructure necessary to dynamically manage the hierarchical mesh framework. Despite this complexity, it is generally believed that future applications will increasingly rely on adaptive methods to study problems at unprecedented scale and resolution. Implementing efficient adaptive meshes in GPU-accelerated systems is significantly hard in comparison to traditional CPU systems. More specifically, GPUs add complexity overhead for managing the mesh hierarchy and optimization of data movement. This is made evident by the relatively wide use of AMR in CPU in comparison to GPU-based systems. For example, a mature AMR framework supporting CPU, namely FLASH is reported to be in use by dozens of production applications [1]. On the contrary, a few number of individual applications adapted AMR solvers for GPU, with varying levels of optimization and scaling. To summarize the problems with GPU-based AMR, only a few frameworks enable automated AMR transformations for GPU, and their programming models require the programmer to write his own versions of the target-optimized solvers. Moreover, there can be scalability limitations caused by the overhead of the CPU-GPU communication schemes in those frameworks [2]. In this work, we present a high-level framework, called Daino [3], which auto-generates efficient and scalable structured AMR solutions to scientific applications running on GPU-accelerated systems.

13.3.2.2 Background

Structured AMR methods use logically rectangular meshes in the implementation of the adaptive mesh. Structured AMR utilizes a hierarchy of levels of spatial, and often temporal, mesh spacing with each level being composed of a union of logically rectangular mesh regions. One way to represent the structured AMR, namely tree-based AMR, divides the discretized domain into fixed blocks. If any cell within a block requires refinement, the whole block is refined. In the tree-based scheme, the mesh is organized into a hierarchy of refinement levels. The mesh is usually decomposed into relatively small fixed-sized octants of mesh cells. Each octant can be recursively refined into a set of octants of fine cells. The mesh configuration is managed using a tree-based data structure that maintains explicit child- parent relationships between coarse and fine octants. Size relations between neighboring octants are typically enforced in structured AMR, which means neighboring octants can have at most one level of refinement difference (referred to as 2:1 balance). An important feature of octrees is that the traversal of an octree across its leaves corresponds to a Morton z-shaped Space Filling Curve (SFC) in the geometric domain [4]. Accordingly, sorting the blocks by their Morton ID and equally partitioning them leads to a uniform distribution of the blocks of a mesh among different Processing Elements (PEs), while benefiting from the locality provided by SFC affinity. Figure 13.4 illustrates how the domain and tree are represented in AMR, and the use of SFC to divide the blocks among three PEs.

13.3.2.3 High-level Framework for Efficient AMR

We design a high-level programming framework that provides a highly productive programming environment for AMR. The framework is transparent and requires minimal involvement from the programmer, while generating efficient and scalable AMR code. The framework consists of a compiler and runtime components. A set of directives allows the programmer to identify stencils of a uniform mesh in an architecture- neutral way. The uniform mesh code is then translated to GPU-optimized parallel AMR code, which is then compiled to an executable. The runtime component encapsulates the AMR hierarchy and provides an interface for the mesh management operations.

Programming Model: The framework provides directives to be used with standard C (details on directives in next section). The programmer is required to add the directives to a serial uniform mesh code in order to identify the operations and stencil data arrays that are the target for transformation. Note that the directives are not changing the uniform mesh implementation; the programmer can still use the uniform mesh implementation if the directives are ignored by compiler.

Optimizations: When an AMR code generated by Daino is executed on a GPU-accelerated cluster, the stencil and mesh adaptation kernels run on the GPU, while managing the octree data structures and load

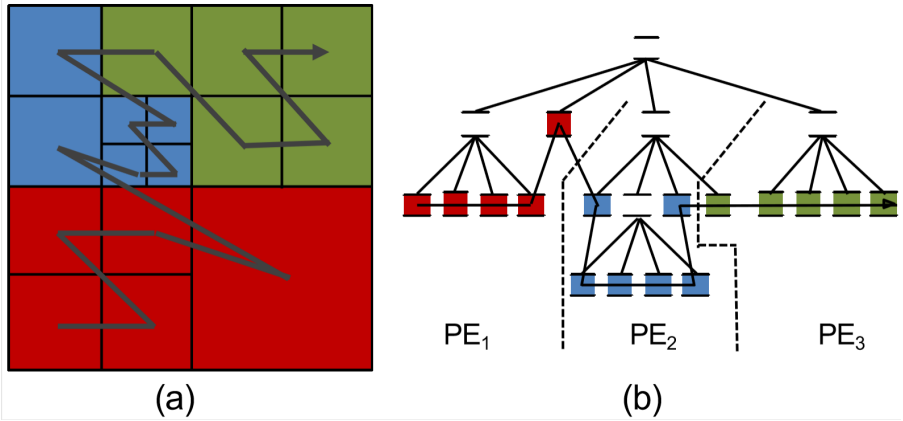

Figure 13.4: Octree-based meshes. The blocks are equally partitioned into three PEs using a space filling curve. (a) Adaptive mesh (b) Tree representation (Note: 2D quadtree is used for illustration)

balancing is done on the CPU side. Since we pursue efficiency and scalability, code on both the CPU and GPU should be optimized. The stencil operations in the blocks are themselves optimized for the GPU architecture [5]. Other optimizations, such as data layout in memory and using user-managed cache memory, are applied on the GPU kernels responsible for adapting the mesh: error estimation, refinement (interpolation), and coarsening (extrapolation). Finally, the generated code includes optimizations to reduce the communication between nodes, i.e. boundary data exchange, and balancing the load, i.e. number of blocks per node.

Implementation: Our framework consists of a compiler and runtime components. We generate executables optimized for GPU execution by leveraging the LLVM compiler infrastructure. The compiler builds on the LLVM compiler infrastructure [6]. First, we use the front end to analyze and translate the stencil source code into GPU-optimized code in the form of LLVM Intermediate Representation (IR). Next, compiler passes are applied on the IR to add the AMR management code, which in turn make API calls to the runtime API and GPU-optimized code generated by the Nvidia backend code generator. Finally, LLVM IR is compiled and linked with the runtime libraries to generate and executable. The runtime includes two libraries, the first library encapsulates the AMR hierarchy management software and the second is a communication library that wraps the MPI runtime library to simplify data movement operations for the AMR driver. The stages of compilation and layout of Diano are shown in Figure 13.5.

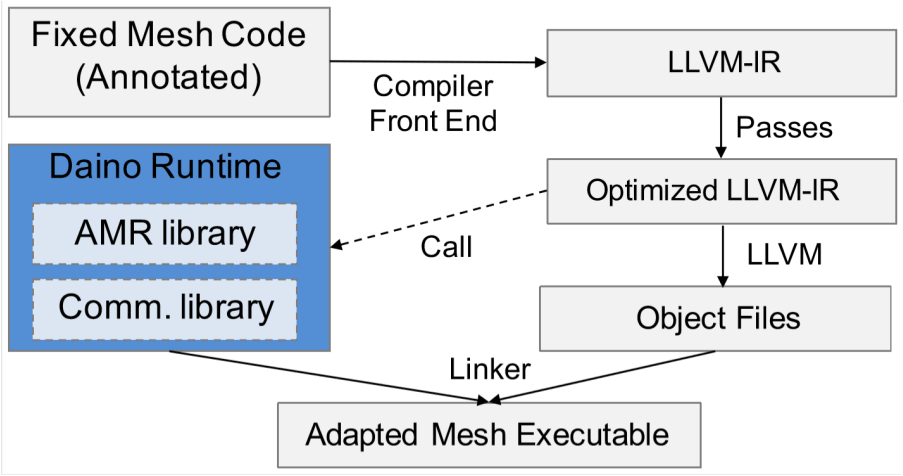

Figure 13.5: The framework overview

13.3.2.4 Evaluation

We demonstrate the scalability of auto-generated AMR code using three production applications. We compare the speedup and scalability with hand-written AMR of all three applications.

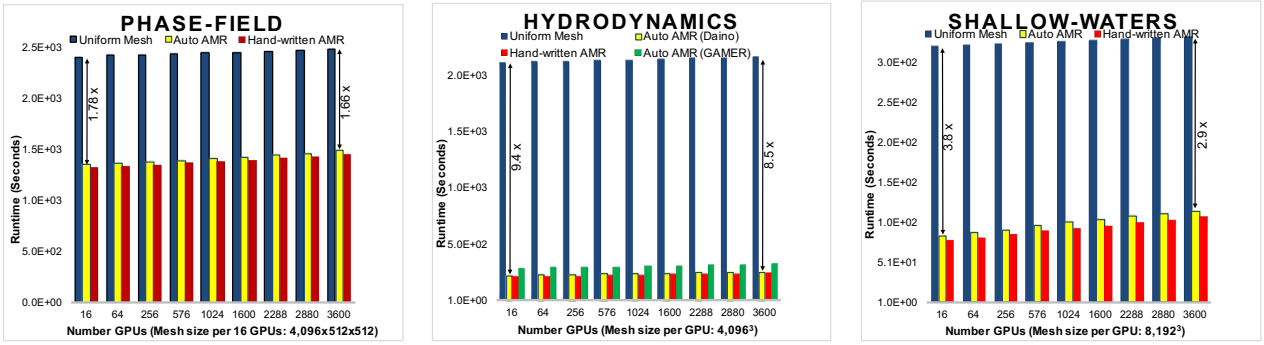

Figure 13.6: Weak scaling of uniform mesh, hand-written and automated AMR

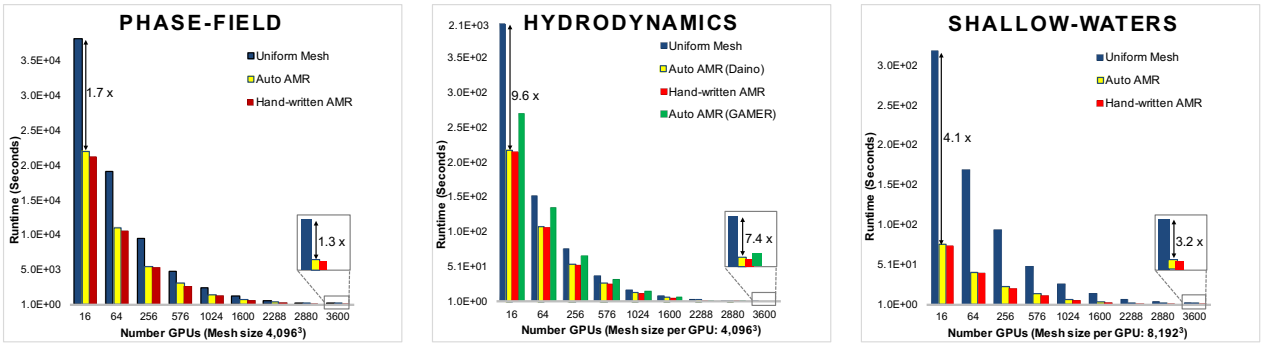

Figure 13.7: Strong scaling of uniform mesh, hand-written and automated AMR

Applications: a) Phase-field Simulation: This application simulates 3D dendritic growth during binary ally solidification [7], b) Hydrodynamics Solver: This solver models a 2nd order directionally split hyperbolic schemes to solve Euler equations [8], and c) Shallow-water: Modeling shallow water by depth-averaging Navier-Stokes equations [9].

Results: In a weak scaling experiment, shown in Figure 13.6, the run- time for uniform mesh, hand-written AMR, and auto-generated AMR are compared. The following points are important to note. First, more than 1.7x speedup is achieved using Daino suing the full TSUBAME machine, 3,640 GPUs, for the phase-field simulation. This is a considerable improvement considering that the uniform mesh implementation is a Gordon Bell prize winner for time-to- solution [7]. Second, Daino achieves good scaling that comparable to the scalability of the hand-written AMR code. Figure 13.7 shows a strong scaling comparison for hand-written and auto-generated AMR against uniform mesh implementation. The code generated by Daino achieves speedups and scalability comparable to hand-written implementations. However, when using more GPUs, reduction in speedup starts to occur as the management of AMR starts to dominate the simulation runtime.

13.3.2.5 Summary

Producing efficient AMR code is a challenge, especially for GPUs. We introduce a framework for producing efficient and distributed AMR code for GPU-accelerated systems. We demonstrated the efficacy and scalability of three applications using the full TSUBAME supercomputer. To the authors knowledge, this is the first study to scale auto-generated AMR code to O(1,000s) of GPUs. However, there are still problems to be solved, for example, handling of customized error functions and boundary conditions.

13.3.2.6 References

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13.3.3 Extending a Global Climate Model with a High Level Framework

Mature climate models are complex codebases comprised of different components each with its own requirements and specifics. As we transition into the complex, and diverse, architectures of next-generation supercomputers, optimizing and adapting each of those components becomes more challenging. An additional challenge is to assure that those optimized components will seamlessly work together, in a performance portable fashion. In this work, we investigate a path for transitioning climate models to next-generation supercomputer, which an emphasize on performance profitability and end-user productivity. More specifically, We aim to demonstrate how to approach and integrate each of the components of an atmospheric model, NICAM. For porting the entire dynamical core, we use a C++ framework developed by the Swiss National Supercomputing Center, named GridTools, that could produce highly performing code for different target architectures. For the physical parameterization component, we propose a user-friendly Python-based approach to assure high productivity and practicality; physical parameterization code is typical continuously changed, unlike the dynamical core. It is important to note is that performance portability is a main concern we try to address in this work; next-generation supercomputers have high diversity in architectures.

13.3.3.1 Porting NICAM-DC 2016 Benchmark

To evaluate the productivity and performance of GridTools, we extracted seven kernels from the dynamical core of NICAM (publicly available at:
`https://github.com/hisashiyashiro/nicam_dckernel_2016`). We found that the performance for three benchmarks is comparable to hand-written CUDA code. Performance in comparison to hand-written OpenMP code for CPU is also found to be satisfactory. Based on the promising results, we continue to port the dynamical core of NICAM to GridTools.

13.4 Schedule and Future Plan

For the scalable multi-granular data model, we plan to improve the implementation to further reduce overhead and apply it to other applications, such as weather prediction. For the global climate model study, we plan to continue the study of the effectiveness of high level frameworks such as GridTools.

13.5 Publications

13.5.1 Journal Articles

13.5.2 Conference Papers

[1] Shinichiro Takizawa, Motohiko Matsuda, Naoya Maruyama, Yoshifumi Nakamura. A Scalable Multi-Granular Data Model for Data Parallel Workflows. HPC Asia 2018. 2018 (submitted).
[2] M. Wahib, N. Maruyama, T. Aoki, Daino: A High-level Framework for Parallel and Efficient AMR on GPUs, SC'16, ACM/IEEE Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (2016)

13.5.3 Posters and Presentations

[3] M. Wahib, Invited Talk: "Daino: A High-level Framework for Parallel and Efficient AMR on GPUs',' Argonne National Laboratory, December 2016 RIKEN AICS (PADAL Workshop)
[4] Shinichiro Takizawa, Motohiko Matsuda, Naoya Maruyama. A Locality-aware Task Scheduling of Message Passing and MapReduce Hybrid Models. HPDC 2016 Poster. 2016.
[5] M. Wahib, Invited Talk: "Automatically Fusing Hundreds of Stencil Kernels for Better Performance and Productivity," GTC 2016 (Nvidia GPU Technology Conference)

Chapter 14

Advanced Visualization Research Team

14.1 Members

Kenji Ono (Team Leader)

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Yukiko Hayakawa (Assistant)

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Aya Mothoshi (Assistant)

14.2 Research Activities

The research and development activities of this team have been focused on the methods, tools, and techniques for the visualization and analysis of large-scale parallel simulation results generated by the K computer. However, the research focus has not been confined to the traditional *post-hoc* visualization and analysis of the stored simulation results, and involves a wide range of topics in the *end-to-end* simulation and visualization pipeline. This wide range of research activities involving both simulation [1][9-14][19], and visualization [2-8][15-18] oriented topics have been helpful for better understanding of issues and challenges inherent to the simulation and visualization, and for trying to provide an optimized solution for the large-scale data visualization and analysis, including an automated scientific workflow system.

In this fiscal year, our team has worked on the enhancements and refinements of *HIVE (Heterogeneously Integrated Visual-analytics Environment)*, a scalable and multi-platform visualization application, which can

run directly on the K computer, and *ChOWDER (Cooperative Workspace Driver)*, a Web-based multi-monitor controller system. These two applications can be utilized separately as independent applications, and also in conjunction to enable a cooperative visual analysis environment by using a multi-screen display system with large dimensions. The *HIVE* was also utilized to provide a large-data visualization ecosystem, and an integration with the *KVS (Kyoto Visualization System)* library has been conducted as a collaborative research with Kyoto University and Kobe University. Envisioning the functionality enhancements of the *HIVE*, our team has also investigated the potential of a novel visual analytics technique, named *Flexible Fiber Surface*, for the visual analysis of multivariate data sets. In addition, other core techniques, for the possible future integration with the *HIVE*, such as compression, parallel image composition, *in-situ* visualization, and VR (Virtual Reality) have also been investigated. our team has also investigated the promising *PinT (Parallel-in-Time)* integration method and the visualization and analysis issues when handling this kind of simulation results.

14.3 Research Results and Achievements

14.3.1 Visual Analytics Framework (HIVE)

The prototype of the *HIVE* framework developed in the previous fiscal year has been refined and enhanced focusing the public release as a production-grade application. Some user feedbacks during the real-world usage, such as during the *AICS Open Source Workshop Program* and *AICS Internship Program*, have been taken into consideration for this refinement process. The front-end Web-based GUI (Graphical User Interface), shown in Figure 14.1, has been completely renewed enabling the dynamic interaction via mouse and keyboard. This interaction includes not only the traditional visual exploration on the rendering window, but also the flexible interaction throughout the GUI workspace for the positioning of modules, windows and module connections [5][15][16].

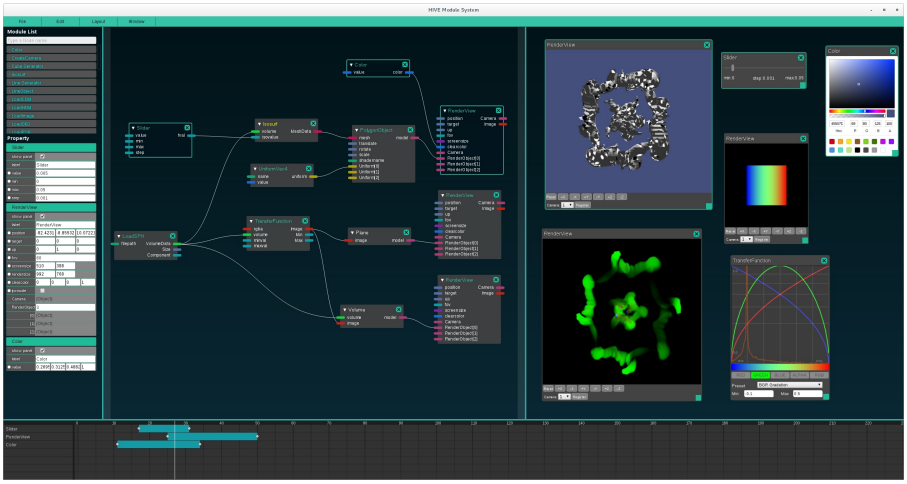


Figure 14.1: The web-based graphical user interface of the HIVE framework, which enables interactive visual exploration via mouse and keyboard.

The parallel image compositor module, *234Compositor*, has been enhanced to enable the *on-site sorting*, for the correct *alpha blending* operation, by taking advantage of the *SURFACE* ray tracing engine which can separately provide the depth information of the pixels [2]. An initial real world usage evaluation of the *HIVE* has been done by using some CFD (Computer Fluid Dynamics) simulation results generated by the K computer [4]. It is worth noting that two sets of high-resolution images generated by the *HIVE* on the K computer have been utilized as 8K4K movies, for the contents transmission demo, during the official Opening Ceremony of the NII SINET 5 (Science Information Network).

The modular and flexible front-end GUI of the *HIVE* has also been used as a large data visualization ecosystem for integrating third party visualization functionalities. An initial trial has been done by integrating the functionalities of the *KVS (Kyoto Visualization System)* scientific visualization library, which is being developed by Kyoto University and Kobe University, and the results can be shown in Figure 14.2 [6][17]. Compression based methods for *in-situ* visualization [8] and flow visualization [9]; a visualization approach by

using portable VR device [18] have also been investigated and evaluated as some potential approaches for the future integration with the *HIVE*.

14.3.2 Scientific Workflow System

Some scientific fields have increasingly required high-throughput and efficient virtual screening infrastructure for the discovery and development processes of new drugs, substances, and materials. In such cases, there are high demands for executing large number of small jobs within a certain period of time, which is known as *Capacity Computing*. In the capacity computing, the workflow of these small jobs usually includes the pre- and post-processing thus the automation of the entire workflow including the data analysis becomes highly important. In order to meet these requirements, our team has worked, in collaboration with a research group in the Kyushu University, on the research and development of a new automated workflow system named *SWF (Scientific WorkFlow)*, which took into consideration the knowledge obtained during the research and development of *HIVE* and *HPC/PF*.

The *SWF* is a multi-platform automated job preparation environment, including pre- and post-processing, for the efficient job execution on the HPC systems. Since the GUI is web-based and operated via web browser thus it does not depend on the executing hardware platform. The main processing is based on *Node.js*, which is a cross-platform runtime environment, and enables its use from the Linux, Mac, and Windows hardware platforms. Users can define the "tasks" for each of the processing units via web-based GUI of the *SWF*, and can define the execution order by connecting these tasks under the GUI workspace, as shown in Figure 14.3.

Detailed processing within each of the tasks can be written by using traditional scripting languages such as Unix Shell Script, Python, and Lua. Flow control structures such as "repetition" and "conditional branching" can also be performed. In addition, a searching parameter space can be defined by using the GUI parameter editor, which is attached to the *SWF*. This editor possesses also a parameter study function that can automatically execute multiple jobs based on the parameter combinations within the parameter searching range. In this fiscal year, the collaborative research team developed a *SWF* prototype, with some basic functions, and evaluated the aforementioned parameter study function by using the Fujitsu PRIMEHPC FX-10 installed at the Kyushu University.

14.3.3 Multi-Monitor Controller System (ChOWDER)

The ever increasing resolution and complexity of modern large-scale simulation has demanded not only a higher resolution visual analysis environment, but also a collaborative discussion and decision making environment during the visual analysis of the numerical simulation results. In order to meet this demand, our team has worked on a web browser based multi-monitor controller system, named *ChOWDER (Cooperative Workspace Driver)*, and was designed to assist collaborative work among multiple users and applications. The development of the *ChOWDER* has been conducted by the financial support of the cross-ministerial Strategic Innovation promotion Program (SIP).

The *ChOWDER* delivers the functionality of virtual display driver for tiled wall display, and can be used for building scalable cooperative workspace environment for designers and engineers as shown in Fig. 14.4. As

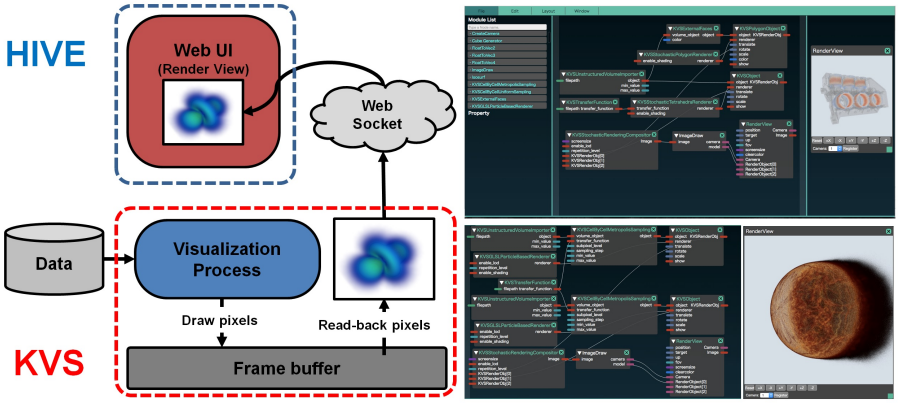


Figure 14.2: The synergistic integration of the HIVE framework (RIKEN AICS) and the KVS visualization library (Kyoto University and Kobe University).

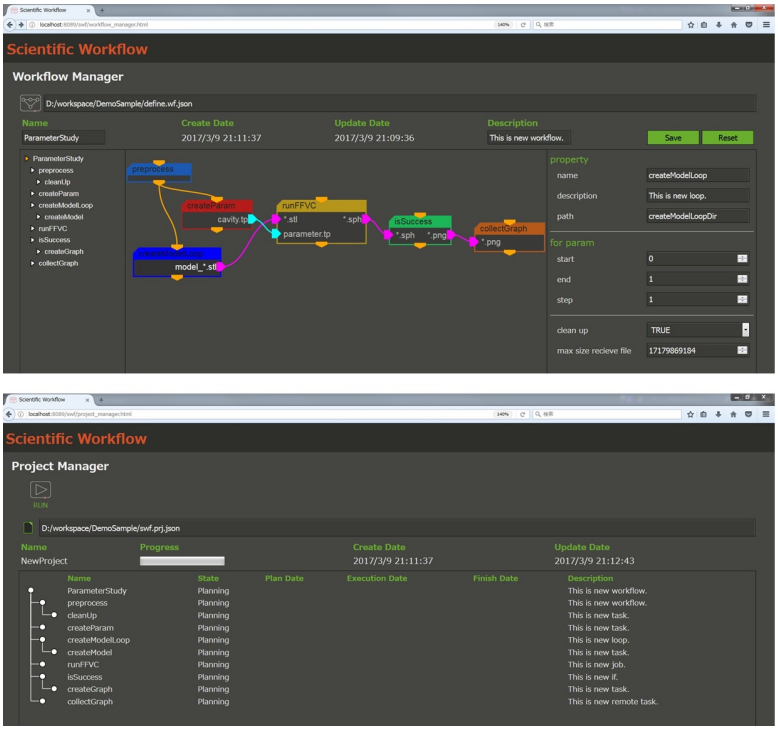


Figure 14.3: An overview of the SWF prototype and its web-based GUI.

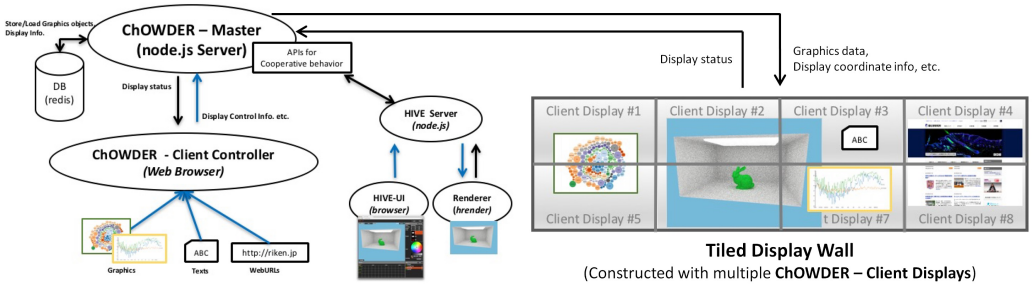


Figure 14.4: An overview of the ChOWDER showing its main components (ChOWDER Master, Client Controller, and Client Displays)

shown in this figure, one of the differentials of the *ChOWDER* is the presence of the "*APIs for Cooperative behavior*", which enables a seamless communication with the *HIVE* for directly displaying the rendering output to the *Client Displays*. As a real world usage, the *ChOWDER* was utilized as a supporting tool for the student trainings and exercises during the Space Education Program at the Tokyo University of Science, and was the first result of the open source strategy for our SIP research theme.

14.3.4 J-Global Data Analysis System

Under the funding of Cross-Ministerial Strategic Innovation Promotion Program (SIP), our team has also developed the *J-Global Data Analysis System* for the JST papers/patents database (Figure 14.5). This system provides a visual analysis tool, which supports the bird's eye view of the research and market trends surrounding a given product development case. As an evaluation of the real world usage, we have applied this data analysis system to the development case of a cyclone separator, which is a device for removing solid particles from air, gas or liquids. This system can be used for general purpose data analysis by simply substituting the input data source as well as the searching database.

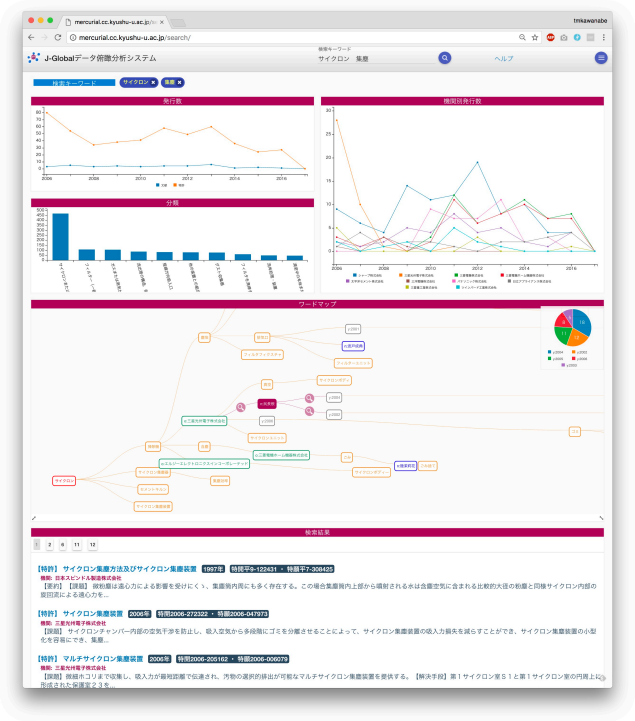


Figure 14.5: An overview of the J-Global Data Analysis System showing its Web-based GUI workspace, and a case study for the “cyclone separator”.

14.3.5 Flexible Fiber Surface

Our team has enhanced the multi-variate visual analysis technique, named *Fiber Surface*, developed in the previous fiscal year, by developing a novel technique that can cluster and track features considering multiple quantities. We composed such features from the intersection of multiple isosurfaces, which respects the convention of traditional data analysis. Our interactive analysis allows a data analyst to visualize how the region of interest distributes in the spatiotemporal domain and to alter the parametrization per cluster interactively as shown in Figure 14.6. The proposed algorithm shall be extended to distributed systems with good scalability. Such scalability is what the existing approaches, primarily topological analysis, fell short. The proposed technique named *Flexible Fiber Surface* was presented at the conference “Topology-Based Methods in Visualization 2017” [7], and we also submitted a full paper to the book series “the Mathematics + Visualization series” from the Springer Verlag [3].

14.3.6 Parallel-in-Time Integration

The *Parallel-in-Time (PinT)* integration method [10][19] is a promising approach to effectively exploit the ever increasing concurrency of the modern HPC systems, and especially to the post peta-scale parallel computing systems which are expected to further increase the current degree of concurrency. The study of *PinT* method has rapidly advanced after the introduction of the *Parareal* method (Figure 14.7(a)) by Lions in the beginning of the 2000s. Therefore, our team has investigated the applicability of the *Parareal* method to the particle tracking, which is one of most important methods in the scientific visualization field. The particle tracking method is based on the time integration of ODE (Ordinary Differential Equation), and our investigation found that the *Parareal* method works well for the ODEs and parabolic PDEs (Partial Differential Equations), but does not work so well for the hyperbolic PDEs, as shown in (Figure 14.7(b)). Therefore, we could conclude that the *Parareal* method is a promising candidate for the time integrator of particle tracking method, and deserves further developments.

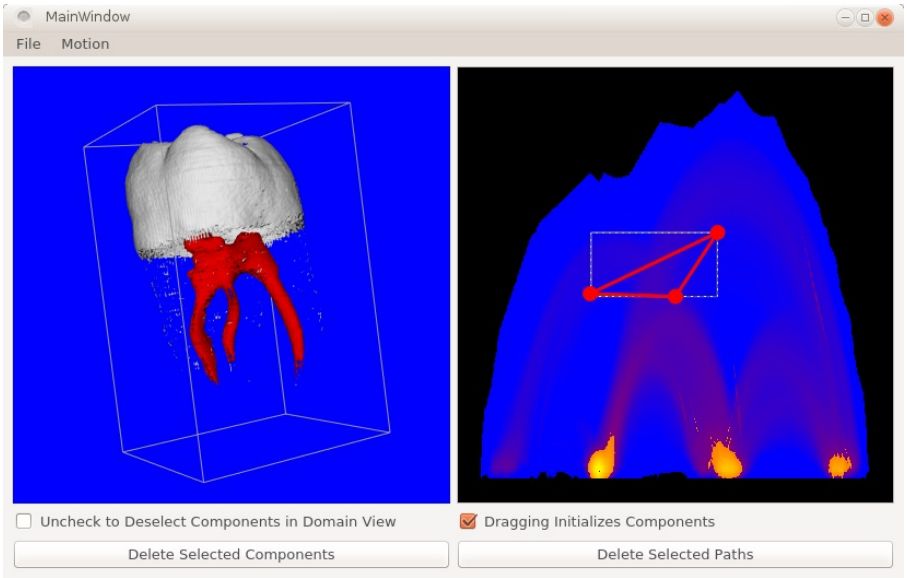
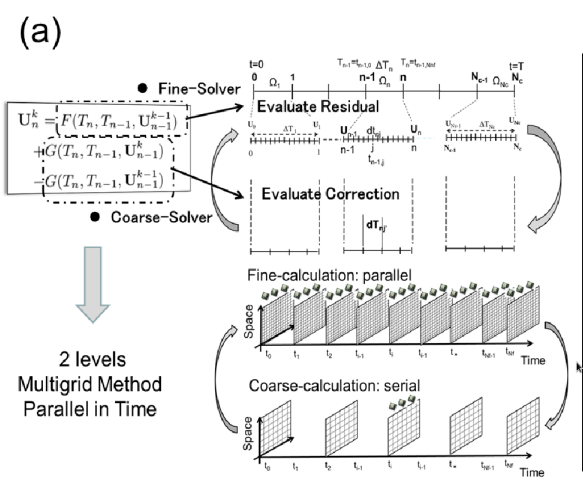


Figure 14.6: Fig 3: The GUI prototype for the Flexible Fiber Surface module.



(b)

Type	Applications	level
ODE	CMD, QMD, Chemical reaction, Hamiltonian system, Nonlinear particle system	Work well
Parabolic PDE	Heat equation, Neutron diffusion transient model, Fusion plasma	Work well
Hyperbolic PDE	Wave equation, Advection equation.	Dose not work

Figure 14.7: (a) An overview of the Parareal algorithm. (b) Applicability table of the Parareal approach to the particle tracking method.

14.4 Schedule and Future Plan

Most of the research and development results in this fiscal year have been integrated as functions or modules to the *HIVE* [20] and *ChOWDER* [21], and released as open source software packages, and continuously updated, through the GitHub code repository. The new version of the *HIVE* and *ChOWDER*, which have been matured to the near production grade applications, have been presented for the potential users in the *AICS Open Source Workshop Program*. In order to verify the potential weakness and future enhancements, we are aware that we need more investigation by utilizing in real world usage scenarios. For this purpose, in the FY2017, the *HIVE* framework is expected to be used in two separate programs of the JHPCN (Joint Usage/Research Center for Interdisciplinary Large-scale Information Infrastructures). Since the target data sets and visualization requirements of these two research programs are different, we are expecting that this will be a grateful chance for evaluating the HIVE in a real world utilization scenario and also on different HPC hardware platforms.

14.5 Publications

14.5.1 Journal Articles

[1] Seigo Imamura, Kenji Ono, and Mitsuo Yokokawa. "Iterative-Method Performance Evaluation for Multiple Vectors Associated with a Large-Scale Sparse Matrix". In: *International Journal of Computational Fluid Dynamics*, doi: 10.1080/10618562.2016.1234046, (2016), pp. 1-7.

[2] Jorji Nonaka, Kenji Ono, and Masahiro Fujita. "234Compositor: A Flexible Parallel Image Compositing Framework for Massively Parallel Visualization Environments". In: *Elsevier Future Generation Computer Systems*, doi:10.1016/ j.future.2017.02.011, (In Press).

[3] Daisuke Sakurai, Kenji Ono, Hamish Carr, Jorji Nonaka, and Tomohiro Kawanabe. "Flexible Fiber Surfaces: A Reeb-Free Approach". In.: *Topological Methods in Data Analysis and Visualization V*, (In Submission).

14.5.2 Conference Papers

[4] Jorji Nonaka, Kenji Ono, Masahiro Fujita, Kentaro Oku, and Tomohiro Kawanabe. "HIVE: A Visual Analytics Framework for Large-Scale CFD on the K Computer". In: *28th International Conference on Parallel Computational Fluid Dynamics (Parallel CFD 2016)*, Kobe, Japan, 2016.

[5] Kenji Ono, Jorji Nonaka, Masahiro Fujita, Kentaro Oku, and Tomohiro Kawanabe. "Development of Large-Scale Parallel Visualization System HIVE". In: *The 21th Workshop of Japan Society for Computational Engineering and Science*, Vol. 21, Niigata, Japan, 2016.

[6] Takashi Shimizu, Naohisa Sakamoto, Jorji Nonaka, Kenji Ono, and Koji Koyamada. "Web-based Visualization System for Large-Scale Volume Datasets" In: *Symposium on Numerical Simulation and Visual Analytics of Nonlinear Problems (held in conjunction with JSST Annual Conference 2016)*, Kyoto, Japan, 2016.

[7] Daisuke Sakurai, Kenji Ono, Hamish Carr, Jorji Nonaka, and Tomohiro Kawanabe. "Flexible Fiber Surface: A Reeb-Free Approach (Extended Abstract)". In: *Topoloby-Based Methods in Visualization 2017 (TopoInVis 2017)*, Tokyo, Japan, 2017.

[8] Chongke Bi, Jorji Nonaka, and Kenji Ono. "Interactive In-Situ Visualization for Large-Scale Simulations". In: *The 3rd China Visualization and Visual Analytics Conference (ChinaVis 2016)*, Changsha, China, 2016.

[9] Fan Hong, Chongke Bi, Hanqi Guo, Kenji Ono, and Xiaoru Yuan. "Compres-sion-based Integral Curve Data Reuse Framework for Flow Visualization". In: *The 3rd China Visualization and Visual Analytics Conference (ChinaVis 2016)*, Changsha, China, 2016.

[10] Mikio Iizuka, and Kenji Ono. "Framework for Building Parallel-in-Time Integration Simulators". In: *The 12th World Congress on Computational Mechanics*, Seoul, Korea, 2016.

[11] Ken Uzawa, and Kenji Ono. "Turbulence Analysis For High Reynolds Number Flow By Open-Source CFD Software FrontFlow/Violet-Cartesian". In: *The 12th World Congress on Computational Mechanics*, Seoul, Korea, 2016.

[12] Ken Uzawa, and Kenji Ono. "Validation of Wall-Modeled LES for High Reynolds Number Flow". In.: *European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS Congress 2016)*, Crete Island, Greece, 2016.

[13] Ken Uzawa, and Kenji Ono. "Parallel Performance of Frontflow/Violet-Cartesian with Wall-Modeled LES Capability". In: *24th International Congress of Theoretical and applied Mechanics(ICTAM)*, Montreal, Canada, 2016.

[14] Akimasa Narita, Keisuke Machida, Saki Egawa, Mizue Munekata, Kenji Ono, Takashi Watanabe, and Hiroyuki Yoshikawa. "Characteristics of Air Flow in a Hemispheric Head Cyclone Separator". *The 27th International Symposium on Transport Phenomena*, Honolulu, USA, 2016.

14.5.3 Posters and Presentations

[15] Jorji Nonaka, Kenji Ono, Chongke Bi, Daisuke Sakurai, Masahiro Fujita, Kentaro Oku, and Tomohiro Kawanabe. "HIVE: A Visualization and Analysis Framework for Large-Scale Simulations on the K Computer (Poster)". In: *9th IEEE Pacific Visualization Symposium (PacificVis 2016)*, Taipei, Taiwan, 2016.

[16] Jorji Nonaka, Kenji Ono, Chongke Bi, Daisuke Sakurai, Masahiro Fujita, Kentaro Oku, and Tomohiro Kawanabe. "HIVE: A Visual Analytics Framework for Massively Parallel Environments (Poster)". In: *11th Computational Science and Visual Analytics Symposium (Kobe University)*, Kobe, Japan, 2016.

[17] Takashi Shimizu, Naohisa Sakamoto, Jorji Nonaka, Kenji Ono, and Koji Koyamada. "Integrated Volume Visualization Environment on the Web (Lightning Presentation)". In: *ISAV 2016: In Situ Infrastructures for Enabling Extreme-scale Analysis and Visualization (held in conjunction with SC16)*, Salt Lake City, USA, 2016.
[18] Jorji Nonaka, Masahiro Fujita, and Kenji Ono. "Walk throuh a Nasal Cavity by using a VR Head Mount Display (Oral Presentation)". *NIFS (National Institute for Fusion Science) Research Meetings for Advanced Visualization Technique*, Toki, Japan, 2016.
[19] Mikio Iizuka, and Kenji Ono. "Investigation of Convergence Characteristics of the Parareal Method for Hyperbolic PDEs using the Reduced Basis Methods". In: *Fifth Parallel-in-time Integration Workshop*, Banff, Canada, 2016.

14.5.4 Patents and Deliverables

[20] *HIVE (Heterogeneously Integrated Visual analytics Environment).* http:// avr-aics-riken.github.io/HIVE
[21] *ChOWDER (Cooperative Work Driver).* https://github.com/SIPupstream Design/ChOWDER

Chapter 15

Data Assimilation Research Team

15.1 Members

Takemasa Miyoshi (Team Leader)

Koji Terasaki (Research Scientist)

Shigenori Otsuka (Research Scientist)

Keiichi Kondo (Postdoctoral Researcher)

Shunji Kotsuki (Postdoctoral Researcher)

Guo-Yuan Lien (Postdoctoral Researcher)

Takumi Honda (Postdoctoral Researcher)

Yohei Sawada (Postdoctoral Researcher)

Atsushi Okazaki (Postdoctoral Researcher)

Toshiki Teramura (Postdoctoral Researcher)

Yasumitsu Maejima (Research Associate)

Hazuki Arakida (Technical Staff)

Gulanbaier Tuerhong (Technical Staff)

Taeka Awazu (Technical Staff)

Hideyuki Sakamoto (Technical Staff)

Juan J. Ruiz (Visiting Scientist)

Shinichiro Shima (Visiting Scientist)

Shu-Chih Yang (Visiting Scientist)

Stephen G. Penny (Visiting Scientist)

Masaru Kunii (Visiting Scientist)

Kozo Okamoto (Visiting Scientist)

Michiko Otsuka (Visiting Scientist)

Marimo Ohhigashi (Research Assistant)

Kenta Kurosawa (Research Assistant)

Arata Amemiya (Intern)

Stefan Geiss (Intern)

Yukie Komori (Assistant)

Rie Deguchi (Assistant)

Kuki Kuniya (Assistant)

Miho Ono (Assistant)

15.2 Research Activities

Data Assimilation Research Team (DA Team) was launched in October 2012 and is composed of 27 research and technical staff including 7 visiting members as of March 2017. Data assimilation is a cross-disciplinary science to synergize computer simulations and real-world data, using statistical methods and applied mathematics. As computers become more powerful and enable more precise simulations, it will become more important to compare the simulations with actual observations. DA Team performs cutting-edge research and development on advanced data assimilation methods and their wide applications, aiming to integrate computer simulations and real-world data in the wisest way. Particularly, DA Team tackles challenging problems of developing efficient and accurate data assimilation systems for "big simulations" with real-world "big data" from various sources including advanced sensors. The specific foci include 1) theoretical and algorithmic developments for efficient and accurate data assimilation, 2) data assimilation methods and applications by taking advantage of the world-leading K computer and "big data" from new advanced sensors, and 3) exploratory new applications of data assimilation in wider simulation fields. These advanced data assimilation studies will enhance simulation capabilities and lead to a better use of the K computer.

In FY2016, we continued on the ongoing data assimilation research in the following aspects: 1) theoretical research on challenging problems, 2) leading research on meteorological applications, 3) optimization of computational algorithms, and 4) exploratory research on wider applications. We also explored close collaborations with several research teams within the AICS Research Division. We have made substantial progress on the following research items:

15.2.0.0.1 Theoretical research

- A new local particle filter method to treat non-Gaussian PDF was explored (1 paper published).
- Non-Gaussian PDF in DA was investigated using the Lorenz-63 3 variable model.
- An object-based verification method of precipitation patterns was investigated using pattern recognition techniques. Incorporating the pattern features in the DA algorithm was also investigated.
- Including the observation error correlation in data assimilation was investigated with the Lorenz96 model. Reconditioning the observation error covariance matrix was found to be effective.
- A particle filter was applied to the cellular automata of 3 state sheep model.

15.2.0.0.2 Leading research on meteorological applications

- Two project-wide papers on the "Big Data Assimilation" experiments for a local severe rainstorm case were published (2 papers published, press release on August 9, 2016).
- The Local Ensemble Transform Kalman Filter (LETKF) system with the SCALE model (SCALE-LETKF) was improved in collaboration with Computational Climate Science Research Team. Several new functions, including observation number limit, integrated observation operator, and static configuration mode, were implemented.
- We continued running the near-real-time regional weather analysis and forecast system based on the SCALE-LETKF on the K computer. It has produced weather analyses and 5-day forecasts every 6 hours for more than 21 months (1 paper published).
- A series of experiments on the Kanto-Tohoku heavy rain event in September 2015 was conducted with the SCALE-LETKF. Various observations including Himawari-8 infrared radiances and dense surface observations provided by NTT DoCoMo were assimilated. River discharge simulations using the SCALE-LETKF precipitation forecasts were conducted.

- Experiments with NHM-LETKF were conducted to investigate an impact of assimilating dense Himawari-8 observations on detecting a local severe storm at an early stage of its development.
- The 3D precipitation nowcasting system with the phased-array weather radar was improved by introducing DA. The computational performance was also improved for the real-time operation. We started a collaboration with MTI Ltd. (press release on 1 March 2017).
- Analyses by the 4-dimensional NHM-LETKF system (4D-NHM-LETKF) were used to investigate the limitation of the linear assumption in convective-scale DA.
- A DA system for JAXA's Global Satellite Mapping of Precipitation (GSMaP) data was developed with Nonhydrostatic Icosahedral Atmospheric Model (NICAM)-LETKF (1 paper published).
- A DA system for Advanced Microwave Sounding Unit (AMSU)-A radiance data with NICAM-LETKF was improved.
- A new adaptive covariance inflation method was developed and applied to the NICAM-LETKF system (1 paper accepted in April 2017).
- A model parameter estimation method was developed with NICAM-LETKF.
- A DA system for Global Precipitation Measurement (GPM) Dual-frequency Precipitation Radar (DPR) was developed with NICAM-LETKF.
- An observing system simulation experiment (OSSE) was conducted with NICAM-LETKF to investigate the impact of including the observation error correlation in the LETKF.
- A DA system without covariance localization in the vertical direction for Advanced Microwave Sounding Unit (AMSU)-A radiance data was developed with NICAM-LETKF.
- Global precipitation nowcasting with the LETKF has been operated in real time using GSMaP (GSMaP RIKEN Nowcast). RIKEN obtained a weather forecasting license from the Japanese Meteorological Agency, and the DA team issues forecasts at https://weather.riken.jp/ (1 paper published).
- Himawari-8 satellite all-sky infrared radiance observations were assimilated with SCALE-LETKF. A case study of Typhoon Soudelor (2015) was conducted.
- A DA system was developed with SCALE-LETKF for a space-borne weather radar in the geostationary orbit. An OSSE was conducted to investigate potential of the geostationary-satellite weather radar.
- Impact of localization in ensemble Kalman filter was investigated with 10,240 samples using an intermediate AGCM (1 paper published).
- An atmosphere-river coupled DA system was developed with NHM-LETKF and a river discharge model. An OSSE assimilating river discharge observation showed a positive impact on the atmospheric variables.
- To improve the accuracy of rainfall and river discharge forecasting with DA, precipitation forecasting experiments were conducted with SCALE. We started collaboration with Tokyo Electric Power Company Holdings, Incorporated. (press release on 15 February 2017)
- We started incorporating a Land DA system into the NICAM-LETKF to assimilate land surface temperature and snow coverage observations measured by satellites. An observation operator for LDA was developed.

15.2.0.0.3 Computational optimization

- The computational performance of the "Big Data Assimilation" problem with the SCALE-LETKF was improved.
- An I/O arbitrator for NetCDF was investigated to accelerate data transfer between SCALE and LETKF in collaboration with System Software Research Team (1 paper published).
- A tree-based geographical search algorithm in the LETKF was implemented in collaboration with Prof. Hideyuki Kawashima's group in the University of Tsukuba.
- The computational performance of NICAM-LETKF was improved in collaboration with Computational Climate Science Research Team (1 paper published).

15.2.0.0.4 Wider applications

- A particle filter was applied to a dynamical vegetation model known as the SEIB-DGVM (Spatially-Explicit, Individual-Based Dynamic Global Vegetation Model). Uncertainties in the state variables and the parameters were greatly reduced by assimilating satellite based Leaf Area Index.
- The SEIB-DGVM DA system was applied to a wider region in the northeastern Eurasia to estimate spatially-varying vegetation parameters.
- A paper on modeling sustainability has been published in collaboration with the University of Maryland (press release on March 13, 2017).

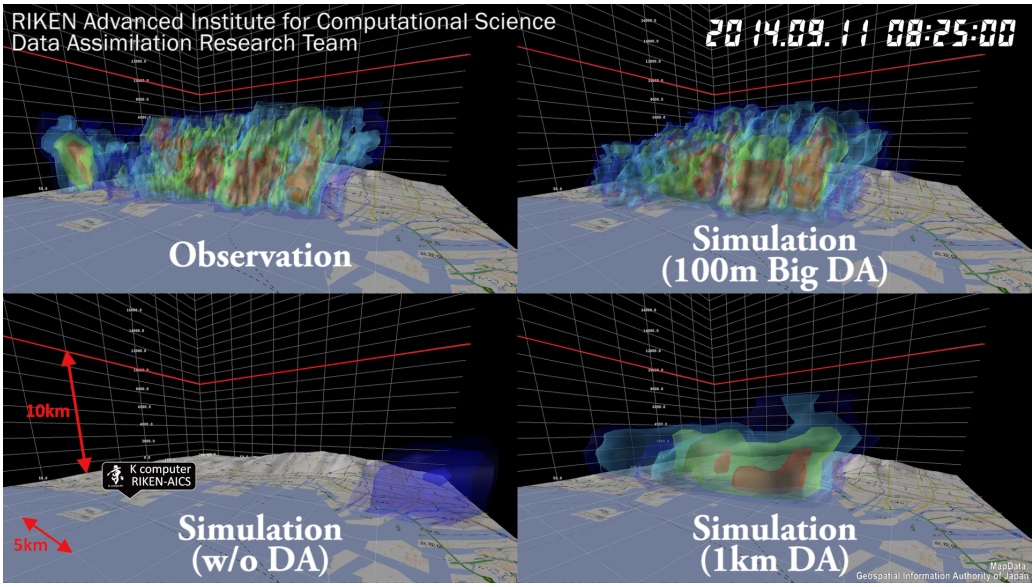


Figure 15.1: Radar reflectivity (dBZ) Top left: real PAWR observation, bottom-left: no data assimilation, top right: 100-m data assimilation, bottom left: 1-km assimilation. Adopted from RIKEN press release on 9 August 2016.

Several achievements are selected and highlighted in the next section.

15.3 Research Results and Achievements

15.3.1 Big Data Assimilation

This research aims to innovate the "Big Data Assimilation" technology for fully taking advantage of big data from Japanese next-generation technologies including the phased array weather radar, next-generation geostationary weather satellite, and world's leading 10-Peta-FLOPS K computer. An innovative 30-second super-rapid update numerical weather prediction system for 30-minute severe weather forecasting will be developed, aiding disaster prevention and mitigation, as well as bringing a scientific breakthrough in meteorology.

Following the achievements in FY2015, we performed data assimilation experiments on the heavy rain event on 13 July 2013 using SCALE-LETKF, with much improvement of the 30-minute forecast accuracy. In addition, we achieved an improvement of computational performance. We also tested the SCALE-LETKF system with other heavy rain cases such as the heavy rain case occurred in Kobe on 11 September 2014. Two project-wide papers were published in FY2016. The first paper, which was submitted to the Bulletin of the American Meteorological Society in FY2015 and accepted for publication on 27 December 2015, was published in August 2016 (Miyoshi et al. 2016). This research result was highlighted by RIKEN Press Release on 9 August 2016 (http://www.riken.jp/pr/press/2016/20160809_1/). The three-dimensional images of the simulation were produced (Fig. 15.1), and they were widely used by newspapers and TV programs. The second project-wide paper was published from the Proceedings of IEEE in November 2016 (Fig. 15.2). This paper summarizes the "Big Data Assimilation" project, experiments on past heavy rainfall cases, computational performance, and future perspectives including real-time operation and use of Himawari-8 observations.

15.3.2 Satellite-based Global Precipitation Data Assimilation with NICAM-LETKF

This study explores an effective use of satellite data including GPM/DPR through an advanced ensemble data assimilation method for improving numerical weather prediction (NWP) and for pioneering a new precipitation product based on an NWP model and satellite observations.

DA Team has been developing a global NWP system known as the NICAM-LETKF (Terasaki et al. 2015). This study assimilates the Japan Aerospace eXploration Agency (JAXA)'s Global Satellite Mapping of Precipitation (GSMaP) data with the NICAM-LETKF. Assimilating precipitation data into numerical models is

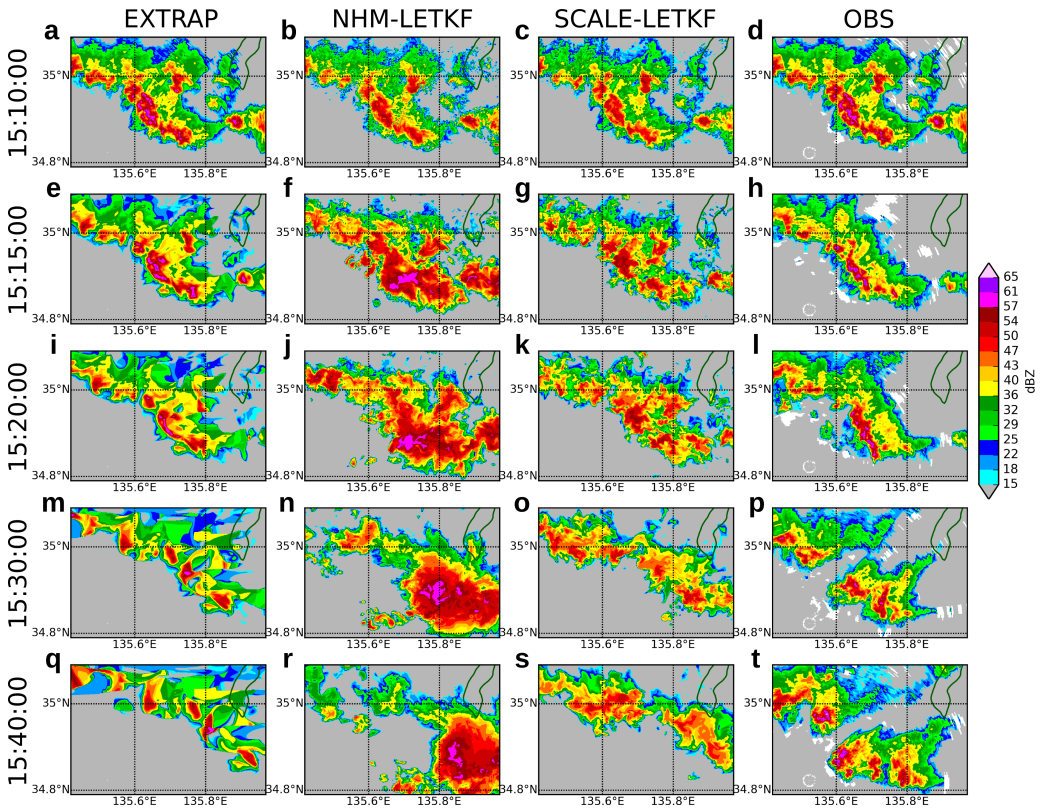


Figure 15.2: Horizontal distribution of radar reflectivity (dBZ) at an elevation angle of 8.125 degrees observed on 13 July 2013. a-d: Initial time (15:10), e-h: 5-min forecasts (15:15), i-l: 10-min forecasts (15:20), m-p: 20-min forecasts (15:30), q-t: 30-min forecasts (15:40). Left: 3D nowcast, Middle-left: NHM-LETKF, Middle-right: SCALE-LETKF, Right: PAWR observations. Adopted from Figure 17 of Miyoshi et al. (2016).

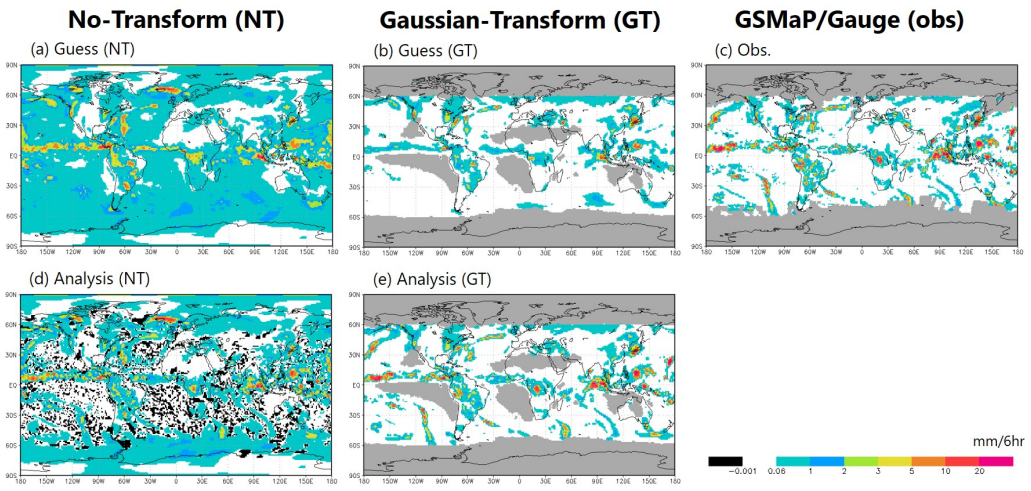


Figure 15.3: Global precipitation patterns (mm 6 h^{-1}) at the first data assimilation step (0000 UTC on 1 November 2014) for (a) NICAM forecast, (b) NICAM forecast after applying the GT, (c) GSMaP_Gauge data, (d) analyzed precipitation without the GT, and (e) analyzed precipitation with the forward and inverse GTs. The gray and black colors show the missing value and the negative precipitation value, respectively. Adopted from Kotsuki et al. (2017).

a difficult problem mainly due to the non-Gaussinan statistics of the precipitation variables and bias between observations and forecasts. Therefore, the assimilation of precipitation data usually results in suboptimal analyses and degraded weather forecasts. Here, we proposed a method to mitigate the non-Gaussian statistics and bias issues by applying the Gaussian transformation (GT) based on past 30-day precipitation data.

Figure 15.3 compares the analyzed precipitation field at the first analysis time. Without the GT (Fig. 15.3d), the analyzed precipitation field contains noisy negative precipitation areas due to the Gaussian error distribution assumption in the EnKF. In contrast, the analysis with GT shows no negative precipitation and becomes closer to the observations (Fig. 15.3e). We extended the experiments, and succeeded to improve NICAM's precipitation forecasts by assimilating the GSMaP. We summarized those findings and published in a high-impact journal (Kotsuki et al. 2017).

15.3.3 Big Ensemble Data Assimilation in Numerical Weather Prediction

We investigated the impact of localization under the perfect model scenario using 10,240 members and intermediate AGCM known as the SPEEDY model (Molteni 2003). The results show that the analysis without localization was greatly improved because of assimilating far distant observations although the ensemble size of 10,240 is much smaller than the degrees of freedom of the SPEEDY model, 133,632. This suggests that the 10,240-member ensemble may be able to estimate the forecast error covariance matrix P^f accurately. Therefore, to investigate the property of P^f, we explicitly compute the eigenvalue decomposition of P^f which has 133,632 eigenvalues, using the efficient eigenvalue decomposition software "EigenExa" (Imamura et al. 2011).

Figure 15.4 shows the eigenvalue spectrum of P^f at after 59 days of data assimilation cycles. The explained variances (EVs) of the first 1,599 and 4,717 principal components are 90.0% and 99.0%, respectively. Moreover, the smallest eigenvalue is about 10^{-5} of the first eigenvalue.

Figure 15.5 shows the first 10 eigenvectors for zonal wind at the 4th model level. The eigenvectors indicate modes with the largest 10 variances among all 10,240 ensemble perturbations, respectively. The signals from the first to fifth eigenvectors mainly appear over the sparsely observed areas (Figs. 15.5a,b,c,d,e). Moreover, some eigenvectors show long range structures even beyond continental scales (e.g., Figs. 15.5f,g,i). This also suggests longer range localization is needed to capture such long-range structures.

15.3.4 Strongly-Coupled Multi-Component Data Assimilation

The Kanto-Tohoku heavy rain in 2015 resulted in a huge damage due to flooding of Kinu River. Hence, flood prediction is important in addition to weather forecasting. Generally, atmospheric observations are assimilated

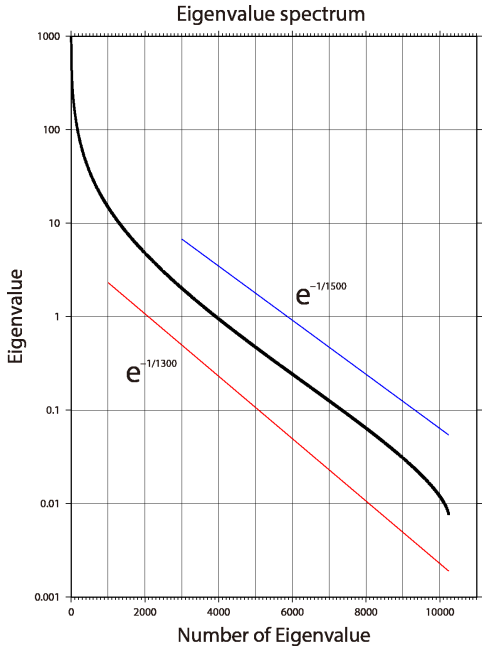


Figure 15.4: Eigenvalue spectrum (black curve) for the forecast error covariance matrix of NOLOC at 0000 UTC 1 March. Red and blue lines indicate e-1/1300 and e-1/1500, respectively. Adopted from Figure 13 of Kondo and Miyoshi (2016).

into an atmospheric model, and precipitation forecasts from the atmospheric model are used as the input to a rainfall-runoff model. On the other hand, river discharge is also observed. Assimilating the river discharge observations to a rainfall-runoff model will help improve the accuracy of flood predictions. In addition, there is a potential that assimilating river discharge observations directly into an atmospheric model will further improve the analysis accuracy of atmospheric variables by using information about in what catchment rainfall occurred. This kind of multiple component data assimilation system is known as a coupled data assimilation system. There are several ways of coupled data assimilation. A weakly coupled data assimilation system assimilates observations independently in each component, and exchanges information via a coupled forecasting system. A strongly coupled data assimilation system assimilates observations by considering cross-component background error covariance. In this study, we developed a strongly-coupled atmosphere-river assimilation system to investigate a potential impact of river discharge observations on the accuracy of atmospheric analyses.

The atmospheric model we used was the JMA-NHM, and the rainfall-runoff model was a simple tank model. Preliminary analyses showed that errors in winds and river discharge were correlated. Here, we performed an observing system simulation experiment. The NHM-LETKF system with 77 members is used, and synthetic observations are generated from a model simulation. Assimilating river discharge observations improved the river discharge as well as the atmospheric variables. Figure 15.6 shows the error reduction in zonal winds, meridional winds, humidity, and precipitation. Atmospheric variables are modified along the rain band over the catchment of Kinu River.

15.4 Schedule and Future Plan

In FY2016, DA team had five additional full-time research staff. We have been working on various aspects of DA including theoretical problems, meteorological applications, and wider applications. “Big Data Assimilation” (BDA) is one of the major activities that we have developed in FY2016. The prototype system showed promising results, but the computing speed with the K computer did not meet the requirement for real-time implementation. Also, the physical performance for the 30-minute forecast of precipitation patterns needs to be improved. We will continue to work on the development of the BDA system to further improve the computational and

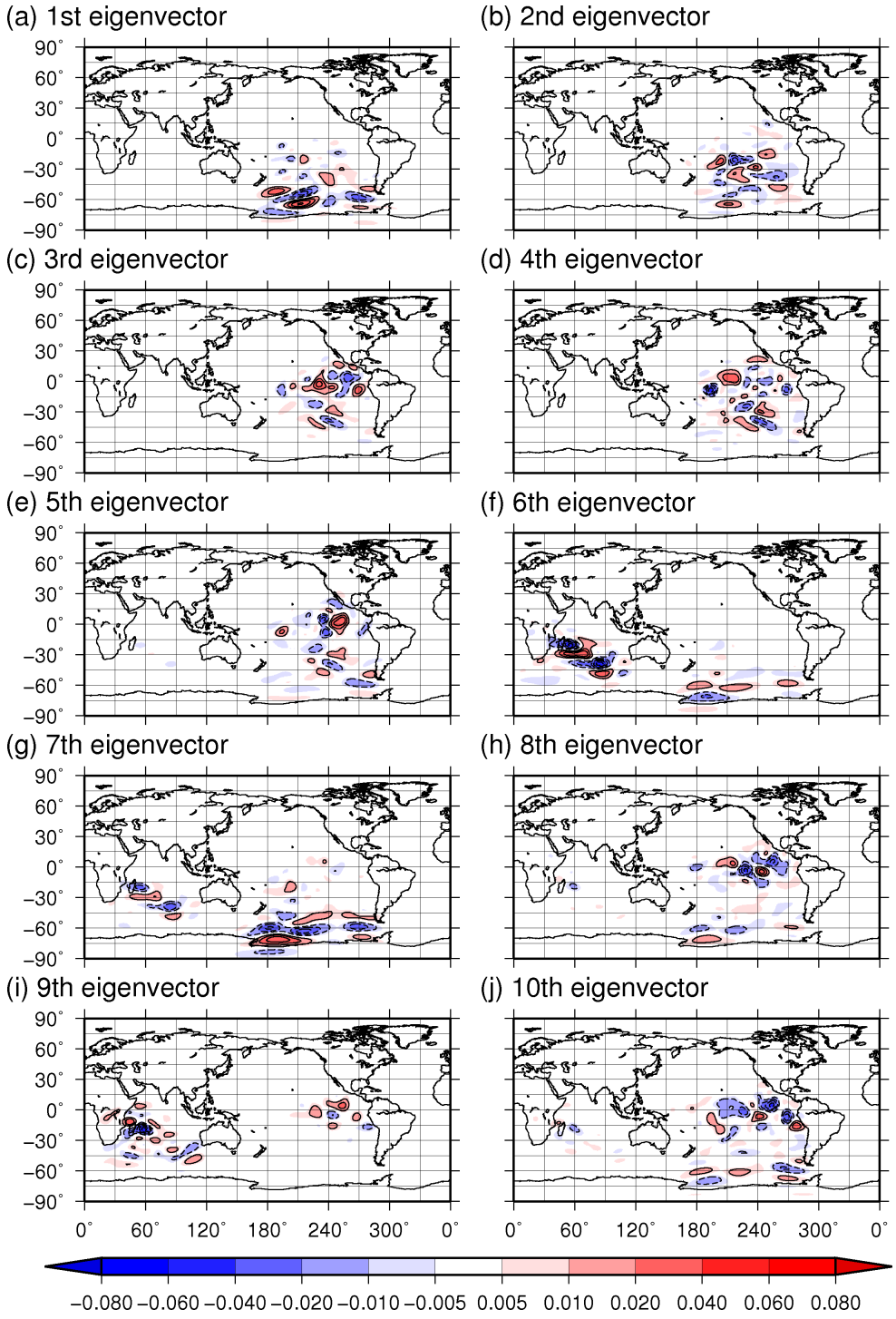


Figure 15.5: The first 10 eigenvectors for zonal wind at the 4th model level at 0000 UTC 1 March. Adopted from Figure 14 of Kondo and Miyoshi (2016).

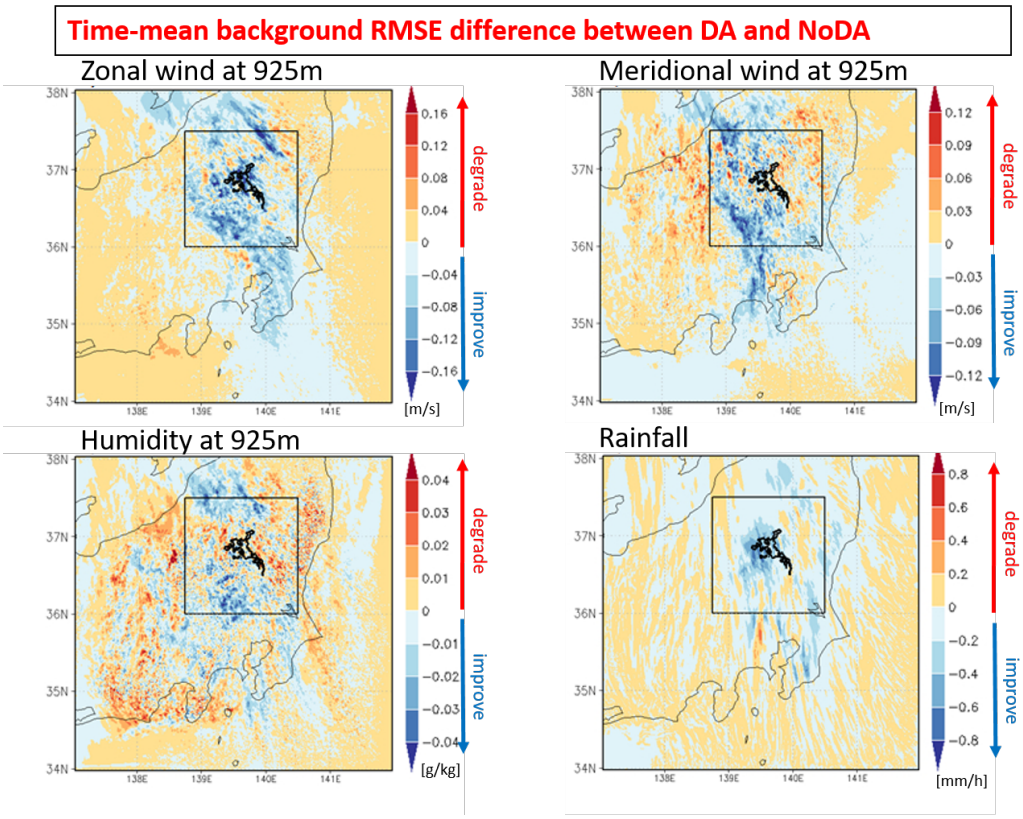


Figure 15.6: Time-mean background RMSE difference of atmospheric variables between experiments with and without assimilation of river discharge observations.

physical performances toward the upcoming "Post-K" era.

Beyond the direct future of the BDA effort, we can extend the idea of BDA to a broader perspective: integration of "Big Data" and "Big Simulation." New sensors provide orders of magnitude more data, and simulations become more precise. Collaborative work with computer scientists will be essential to utilize the complex high-performance computer system effectively. In addition, dense sensor data tend to have correlated errors, and the proper treatment is necessary to fully utilize the "Big Data." The current DA methods commonly assume no correlation in the observation errors. Based on our previous theoretical research on the observation-error correlations, we plan to develop methods to consider the observation error correlations in realistic NWP applications. This is also relevant to satellite data assimilation. The current NWP systems use only a small fraction of available data partly because of the observation error correlations.

Treating the model errors and non-Gaussian probability distribution has been grand challenges in DA. Big Ensemble Data Assimilation with the largest-ever 10,240 samples was a milestone providing fundamental data to investigate the non-Gaussian probability distribution. We have developed expertise and exclusive dataset to tackle these challenges.

For further enhancing our research activities, collaborations with other AICS teams, RIKEN-wide partner (iTHES/iTHEMS), MOU partners (University of Maryland, University of Reading), domestic and international research partners (NICT, Osaka University, JMA, Meteorological Satellite Center, Meteorological Research Institute, Kyoto University, Argentinean National Meteorological Service, University of Buenos Aires, Barcelona Supercomputing Center, LMU Munich , University of Tokyo, Taiwan National Central University, Pennsylvania State University, University of California Davis, JAXA, JAMSTEC, Tokyo Institute of Technology, University of Tsukuba), and industry partners (Tokyo Electronic Power Company, Meisei Electric, MTI) will be the key to success.

In FY2016, we started a new project, DA innovation hub, to expand our activity to wider fields and to attract more people in experimental sciences, computational sciences, and theoretical sciences. We organized the iTHES DA school, RIKEN Inter-disciplinary DA Workshop, RIKEN DA Camp, and the 3rd RIKEN International Symposium on Data Assimilation (RISDA2017). In FY2017, we will continue the DA-Hub project to further seek for new collaborations and seeds of new DA applications.

15.5 Publications

15.5.1 Awards

[1] 2016 年度日本気象学会賞. 三好建正, アンサンブルカルマンフィルタによる データ同化の高度化に関する研究, 2016/5/19

[2] The Most Accessed Paper Award 2016 by Japan Geoscience Union. Satoh, M., H. Tomita, H. Yashiro, H. Miura, C. Kodama, T. Seiki, A. Noda, Y. Yamada, D. Goto, M. Sawada, T. Miyoshi, Y. Niwa, M. Hara, T. Ohno, S. Iga, T. Arakawa, T. Inoue, H. Kubokawa, 2014: The non-hydrostatic icosahedral atmospheric model: description and development. Progress in Earth and Planetary Science, 1:18. doi:10.1186/s40645-014-0018-1, 2016/5/22

[3] Editor's Award, T. Miyoshi, Monthly Weather Review by American Meteorological Society, 2017/1

15.5.2 Journal Articles

[1] Schraff, C., Reich, H., Rhodin, A., Schomburg, A., Stephan, K., Periez, A. and Potthast, R., Kilometre-scale ensemble data assimilation for the COSMO model (KENDA). Q.J.R. Meteorol. Soc., 142, 14531472

[2] Yashiro, H., Terasaki, K., Miyoshi, T., and Tomita, H., Performance evaluation of a throughput-aware framework for ensemble data assimilation: the case of NICAM-LETKF, Geosci. Model Dev., 9, 2293-2300

[3] Sawada, Y., and T. Koike, Towards ecohydrological drought monitoring and prediction using a land data assimilation system: a case study on the Horn of Africa drought (20102011), J. Geophys. Res. Atmos., 121, 8229-8242

[4] Takemasa Miyoshi, Masaru Kunii, Juan Ruiz, Guo-Yuan Lien, Shinsuke Satoh, Tomoo Ushio, Kotaro Bessho, Hiromu Seko, Hirofumi Tomita, and Yutaka Ishikawa, "Big Data Assimilation" Revolutionizing Severe Weather Prediction. Bull. Amer. Meteor. Soc., 97, 13471354

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[6] Otsuka, S., S. Kotsuki, and T. Miyoshi, Nowcasting with data assimilation: a case of Global Satellite Mapping of Precipitation, Weather and Forecasting, 31, 1409-1416

[7] Liao, J., B. Gerofi, G.-Y. Lien, S. Nishizawa, T. Miyoshi, H. Tomita and Y. Ishikawa, Toward a General I/O Arbitration Framework for netCDF based Big Data Processing. Proceedings of the 22nd International Conference on Euro-Par 2016: Parallel Processing - Volume 9833, Pages 293-305

[8] Sawada, Y. and T. Koike, Ecosystem resilience to the Millennium drought in southeast Australia (2001-2009), J. Geophys. Res. - Biogeosci., 121, 2312-2327

[9] Takemasa Miyoshi, Guo-Yuan Lien, Shinsuke Satoh, Tomoo Ushio, Kotaro Bessho, Hirofumi Tomita, Seiya Nishizawa, Ryuji Yoshida, Sachiho A. Adachi, Jianwei Liao, Balazs Gerofi, Yutaka Ishikawa, Masaru Kunii, Juan Ruiz, Yasumitsu Maejima, Shigenori Otsuka, Michiko Otsuka, Kozo Okamoto, and Hiromu Seko, "Big Data Assimilation" Toward Post-Petascale Severe Weather Prediction: An Overview and Progress, in Proceedings of the IEEE, vol. 104, no. 11, pp. 2155-2179

[10] Stephen G. Penny, Takemasa Miyoshi, A local particle filter for high-dimensional geophysical systems, Nonlin. Processes Geophys., 23, 391-405

[11] Kondo, K., T. Miyoshi, Impact of Removing Covariance Localization in an Ensemble Kalman Filter: Experiments with 10 240 Members Using an Intermediate AGCM. Mon. Wea. Rev., 144, 48494865

[12] Lien, G.-Y., T. Miyoshi, S. Nishizawa, R. Yoshida, H. Yashiro, S. A. Adachi, T. Yamaura, and H. Tomita, The near-real-time SCALE-LETKF system: A case of the September 2015 Kanto-Tohoku heavy rainfall. SOLA, 13, 16

[13] S. Kotsuki, T. Miyoshi, K. Terasaki, G.-Y. Lien, and E. Kalnay, Assimilating the global satellite mapping of precipitation data with the Nonhydrostatic Icosahedral Atmospheric Model (NICAM), Journal of Geophysical Research: Atmospheres, 122, 1-20

15.5.3 Conference Papers

15.5.4 Invited Talks

[1] 三好 建正, "Big Data Assimilation" revolutionaizing weather prediction, JST-NSF Big Data Joint Workshop, 東京, 2016/5/11

[2] 三好 建正, 日本気象学会受賞記念講演 "続 $1+1>2$", 日本気象学会 2016 年度春季大会, 東京, 2016/5/19

[3] Keiichi Kondo, Takemasa Miyoshi, "Non-Gaussian statistics and data assimilation in the global atmospheric dynamics with 10240-member ensemble Kalman filter", Japan Geoscience Union Meeting 2016, Chiba, 2016/5/22

[4] 三好 建正, データ同化の進展と広がり, 日本地球惑星科学連合 (JpGU) 2016 年連合大会, 千葉, 2016/5/22

[5] T. Miyoshi, "Big data assimilation" Revolutionizing weather prediction, Symposium on Advanced Assimilation and Uncertainly Quantification in BigData Research for Weather, Climate and Earth System Monitoring and Prediction, State College, Pennsylvania, USA, 2016/5/24

[6] 三好 建正, スーパーコンピュータ「京」が拓く天気予報の未来, 第 155 回制 御技術部会大会（日本鉄鋼協会）, 神戸, 2016/6/16

[7] T. Miyoshi, "Big Data Assimilation" revolutionaizing weather prediction, International HPC Summer School 2016, Ljubljana, Slovenia, 2016/6/29

[8] T. Miyoshi, 'Big Data perspective on assimilating dense observations with spatially correlated errors' RMetS/NCAS Conference 2016 High Impact Weather and Climate, Manchester, UK, 2016/7/6

[9] T. Miyoshi, 'Big Data, Supercomputing, and Data Assimilation', Data Assimilation Research Centre Meetings, Reading, UK, 2016/7/11

[10] G.-Y. Lien, LETKF assimilation of dense radar data for short-range, fine-scale prediction of convective systems, Department of Atmospheric Sciences, National Taiwan University, Taiwan, 2016/7/12

[11] 三好建正, 「ビッグデータ同化」の技術革新の創出によるゲリラ豪雨予測の 実証, CREST「ビッグデータ応用」国際シンポジウム, 東京, 2016/8/5

[12] 三好建正, アンサンブルカルマンフィルタの基礎と応用、「京」を使った最 先端研究の紹介, 海洋データ夏の学校, 青森県むつ市, 2016/8/22

[13] G.-Y. Lien, Assimilation of phased array radar data for short-range NWP using the SCALE-LETKF regional data assimilation system, Research Center for Environmental Changes, Academia Sinica, Taiwan, 2016/10/11

[14] Okazaki, A., Basics of data assimilation and its application to paleoclimate, Kongju National University, Gongju, Korea, 2016/10/20

[15] 荒木田葉月, シミュレーションと衛星観測の融合で地球上の森を再現する, 計算科学連携センター第 3 回学術会議, 神戸, 2016/11/1

[16] 三好建正, スーパーコンピュータ「京」を使った最先端の天気予報アンサ ンブルデータ同化研究, 第 30 回日本計算機統計学会シンポジウム, 沼津, 2016/11/25

[17] 三好建正, 「ビッグデータ同化」で天気予報を革命する, 第 28 回コンピュータシステム・シンポジウム (ComSys2016), 東京, 2016/11/29

[18] Sawada, Y., Towards monitoring and predicting mega-droughts: A model-data integration approach, Future Earth International Co-Design Workshop Earth Observation in Support of the Sustainable Development Goals, Tokyo, Japan, 2017/1/16

[19] 小槻峻司, 三好建正, 予測モデルのためのデータ同化, PSTEP 研究集会, 名 古屋, 2017/1/27

[20] T. Miyoshi, Data Assimilation Research Team, Goals and Activities, Weather-Chaos Meeting, College Park, Maryland, USA, 2017/1/30

[21] T. Miyoshi, 【Keynote】Big Data Assimilation For Extreme-scale Numerical Weather Prediction, BDEC China, Wuxi, China, 2017/3/9

[22] 大塚成徳, ビッグデータ同化：未来の天気予報へ, 豊橋技術科学大学　平成 28 年度計算技術科学実践教育プログラム　最先端データサイエンス講座, 豊 橋, 2017/3/13

[23] T. Miyoshi, Data Assimilation Research at RIKEN: Numerical Weather Prediction and Beyond, AOSC Seminar, College Park, Maryland, USA, 2017/3/16

15.5.5 Oral Presentations

[1] T. Honda, G. Y. Lien, S. Nishizawa, R. Yoshida, S. A. Adachi, K. Terasaki, K. Okamoto, H. Tomita, K. Bessho, T. Miyoshi, Assimilating Himawari-8 Brightness Temperature: A Case Study on Typhoon Soudelor (2015), American Meteorological Society 32nd Conference on Hurricanes and Tropical Meteorology, San Juan, PR, 2016/4/19

[2] 三好建正, 観測ビッグデータを活用するための“ビッグデータ同化”システ ム, ポスト「京」重点課題 4 サブ課題 A 研究連絡会, 東京, 2016/4/21

[3] 寺崎康児, 小槻峻司, 三好建正、NICAM-LETKF の開発状況とコデザイン, ポスト「京」重点課題 4 サブ課題 A 研究連絡会, 東京, 2016/4/21

[4] 三好建正, Enhancing Data Assimilation of GPM Observations, NICAMLETKF and Satellite DA Mtg, 神戸, 2016/4/25

[5] 小槻峻司，寺崎康児, Lien Guo-Yuan, 三好建正，Kalnay Eugenia, NICAMLETKF を用いた全球降水マップ GSMaP のアンサンブルデータ同化実験， 日本気象学会 2016 年度春季大会, 東京, 2016/5/18

[6] 前島康光、国井勝、Juan J. Ruiz, 呉宏堯、佐藤香枝、三好建正 局地的豪雨 予測における高頻度地上観測データ同化のインパクト, 日本気象学会 2016 年度春季大会, 東京, 2016/5/18

[7] 近藤圭一，三好建正, 10240 メンバーのアンサンブルデータ同化実験に基 づいた大気の非ガウス性の調査, 日本気象学会 2016 年度春季大会, 東京, 2016/5/18

[8] 大塚成徳, 三好建正, フェーズドアレイ気象レーダを用いた三次元降水補 外予測の実時間実行に向けた検討, 日本気象学会 2016 年度春季大会, 東京, 2016/5/18

[9] 本田匠, Guo-Yuan Lien, 西澤誠也, 吉田龍二, 足立幸穂, 寺崎康児, 岡本幸 三, 富田浩文, 別所康太郎, 三好建正, ひまわり 8 号輝度温度観測のデータ 同化研究：台風 Soudelor (2015), 日本気象学会 2016 年度春季大会, 東京, 2016/5/18

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[11] Shunji Kotsuki, K. Terasaki, G-Y. Lien, T. Miyoshi, E. Kalnay, Ensemble Data Assimilation of GSMaP precipitation into the Nonhydrostatic Global Atmospheric Model NICAM, Japan Geoscience Union Meeting 2016, Chiba, 2016/5/22

[12] M. KUNII, J. RUIZ, G.-Y. LIEN, T. USHIO, S. SATOH, K. BESSHO, H. SEKO, T. MIYOSHI, Data assimilation experiments of phased array weather radar with 30-second-update ensemble Kalman filter with 100-m resolution, Japan Geoscience Union Meeting 2016, Chiba, 2016/5/22

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[14] Maejijma Y., M. Kunii J, J. Ruiz, H., Kure, K. Sato and T. Miyoshi: Impacts of dense and frequent surface observations on a sudden severe rainstorm forecast: A case of an isolated convective system, Japan Geoscience Union Meeting 2016, Chiba, 2016/5/23

[15] Koji Terasaki, Satellite data assimilation using NICAM-LETKF, Japan Geoscience Union Meeting 2016, Chiba, 2016/5/23

[16] Keiichi Kondo, Takemasa Miyoshi, “Non-Gaussian statistics and data assimilation in the global atmospheric dynamics with 10240-member ensemble Kalman filter”, the 7th EnKF Data Assimilation Workshop, State College, PA, USA, 2016/5/26

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[19] 三好 建正, Enhancing Data Assimilation of GPM Observations, JAXA PMM 8th サイエンスチーム会合, 東京, 2016/6/1

[20] 三好 建正, 理研の同化研究の状況・計画, 「気候システム・放射課程」キッ クオフミーティング（JAXA), 東京, 2016/6/8

[21] 三好 建正, スーパーコンピュータ「京」が拓く天気予報の未来, 理研理事長 定例記者懇談会, 東京, 2016/6/24

[22] Michiko Otsuka, Masaru Kunii, Hiromu Seko, Kazuki Shimoji, ASSIMILATION EXPERIMENTS OF HIMAWARI-8 RAPID SCAN ATMOSPHERIC MOTION VECTORS, 13th International Winds Workshop, Pacific Grove, CA, USA, 2016/6/29

[23] Keiichi Kondo and Takemasa Miyoshi, Non-Gaussian statistics and data assimilation in the global atmospheric dynamics with 10240-member ensemble Kalman filter, THE 5TH ANNUAL INTERNATIONAL SYMPOSIUM ON DATA ASSIMILATION, University of Reading, UK, 2016/7/19

[24] T. Miyoshi, “Big Data Assimilation”: Progress and Plans, ISDA2016, Reading, UK, 2016/7/19

[25] 三好 建正, 「京」と最新鋭気象レーダを生かしたゲリラ豪雨予測—「ビッグ データ同化」を実現、天気予報革命へ—, 記者発表, 東京, 2016/8/1

[26] 小槻峻司，三好建正，寺崎康児, Lien Guo-Yuan, Kalnay Eugenia, NICAMLETKF を用いた全球衛星観測降水データの同化実験，衛星シュミレータ研 究会, 柏, 2016/8/9

[27] 三好 建正, Enhancing Data Assimilation of GPM Observations, NICAMLETKF and Satellite DA Mtg, 神戸, 2016/8/18

[28] 小槻峻司，寺崎康児, 八代尚，富田浩文, 佐藤正樹, 三好建正, 全球衛星観測 降水マップ GSMaP を用いた NICAM のモデルパラメータ推定，GSMaP 研 究会, 大阪, 2016/9/6

[29] 三好 建正, アンサンブル・カルマンフィルタ, iTHES データ同化スクール, 神戸, 2016/9/12

[30] 近藤圭一, 三好建正, 大規模アンサンブルデータ同化実験に基づいた大気 の非ガウス性とその影響, 第 6 回 理研・京大合同データ同化研究会, 神戸, 2016/9/14

[31] 粟津妙華, 大塚成徳, 三好建正, 画像処理技術を用いた降水予測の検証手法, 第 6 回 理研・京大合同データ同化研究会, 神戸, 2016/9/14

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[35] 三好 建正, “Big Data Assimilation” Revolutionizing Severe Weather Prediction, 理研データ同化ワークショップ, 神戸, 2016/10/14

[36] Yeon Joo Lee, IMAMURA Takeshi, SUGIYAMA Ko-ichiro, Sato Takao, Yasumitsu MAEJIMA, Equatorial cloud level convection on Venus, DPS48/EPSC11, Pasadena, CA, USA, 2016/10/21

[37] 小槻峻司, 太田洋一郎, Lien Guo-Yuan, 三好建正, アンサンブルカルマン フィルタの適応型共分散緩和手法, 日本気象学会 2016 年度秋季大会, 名古 屋, 2016/10/26

[38] 澤田洋平, 岡本幸三, 国井勝, 三好建正, ひまわり 8 号を活かした局地的大雨の 予測精度向上の試み, 日本気象学会 2016 年度秋季大会, 名古屋, 2016/10/26

[39] 近藤圭一, 三好建正, 10240 メンバーアンサンブルデータ同化 による局所化 の解析誤差への影響, 日本気象学会 2016 年度秋季大会, 名古屋, 2016/10/26

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[41] 寺崎康児, 三好建正, 観測誤差相関を考慮したデータ同化手法の開発, 日本 気象学会 2016 年度秋季大会, 名古屋, 2016/10/26

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Chapter 16

Computational Disaster Mitigation and Reduction Research Unit

16.1 Members

Muneo Hori (Unit Leader)

Hideyuki Ohtani (Research Scientist)

Jian Chen (Research Scientist)

Kohei Fujita (Postdoctoral Researcher)

16.2 Research Activities

Computational Disaster Mitigation and Reduction Research Unit is aimed at developing advanced large-scale numerical simulation of natural disasters such as an earthquake, tsunami and heavy rain, for Kobe City and other urban areas in Hyogo Prefecture. Besides for the construction of a sophisticated urban area model and the development of new numerical codes, the unit seeks to be a bridge between Science and Local Government for the disaster mitigation and reduction.

The year of 2016 is the final year of the COE project. Our research unit has finalized the core research objectives as well as made preparation of launching a new research objective, as follows:
1) Construction of next generation hazard map for four cities in Hyogo Prefecture. For two scenarios of Nankai Trough Earthquake presumed by National Government, the unit constructed next generation hazard map for four cities in Hyogo Prefecture. Unlike a conventional one, the next generation hazard map is based on large scale numerical simulation of the physical processes of seismic wave propagation and seismic structural responses. The map achieves highest spatial resolution as well as higher rationality. Urban area models of these four cities for man-made structures are used in the physical simulation, and it is these models that determine the quality of the simulation; a more accurate model makes a more reliable estimation of earthquake hazard and disaster. Computational Disaster Mitigation and Reduction Research Unit develops a system called Data Processing Platform that automatically constructs the urban area models using available data resources such as commercial Geographical Information System and governmental data. The system is designed to have high flexibility and expandability so that it can be used for various urban area to which suitable data resources are available.
2) Development of system for real-time estimate of liquefaction occurrence in Hyogo Prefecture. Due to complicated processes, the liquefaction occurrence ought to be estimated by empirical equations that use engineering indices of soil layers of a target site. Computational Disaster Mitigation and Reduction Research Unit constructs a system that enables us to make real-time estimation of liquefaction occurrence; it completes numerical simulation of liquefaction occurrence for 10,000 sites in Hyogo Prefecture for given ground motions. The numerical simulation is made for coupling of soil deformation and underground water flow induced by ground motion, and uses an analysis model for undergrounds that is automatically made by using available boring hole data. Data Processing Platform is used for the automated construction of these underground models.

Figure 16.1: Example of next generation hazard map for Akashi City

3) Study on high fidelity model simulation for natural hazard and disaster. While most advanced numerical simulations are made for the estimation of natural hazard and disaster, it is necessary to increase the accuracy and reliability of the estimation by improving the numerical analysis method that is used for the simulation. To this end, Computational Disaster Mitigation and Reduction Research Unit seeks a high-fidelity model simulation, a massive numerical analysis of a most realistic model of ultra large degree-of-freedom. Such a simulation needs a more advanced numerical analysis method and a better automated model construction. For an exa-scale machine, the analysis method and the construction are being developed.

16.3 Research Results and Achievements

16.3.1 Construction of next generation hazard map for Hyogo Prefecture

National Government issued a possible scenario of Nankai Trough Earthquake. Large and extremely large scenarios were announced for the preparation of earthquake disaster, and a distribution of ground motion index (such as seismic index or peak ground acceleration / velocity) and residential building damage was made by using simple numerical analysis and empirical equations. The distribution is summarized as a hazard map for relatively large "mesh" or "grid" of more than 500 m or town-wise number of damaged houses.

Computational Disaster Mitigation and Reduction Research Unit constructs next generation hazard map for Akashi, Ashiya, Nishinomiya and Amagasaki Cities, using the two presumed scenarios of National Government; see Fig. 16.1 ; the unit has constructed next generation hazard map for Kobe City in 2016. Unlike the conventional hazard map, the next generation hazard map takes advantage of large scale numerical simulation[21-23] of the two physical processes, namely, the seismic wave propagation / amplification and the seismic structural responses. A key issue is the use of Data Processing Platform that constructs analysis models of these two processes for the four cities as shown in Fig. 16.2 . The robustness of the platform is demonstrated as it succeeds to constructs these four models.

Data Processing Platform has a wide range of application since it is able to construct various analysis models for one structure or one city. As an example, we conduct so-called sensitivity analysis of seismic structural response analysis[7], by constructing building analysis models of different structural properties. Data Processing Platform readily constructs normal and week models for each residential building; week models are for the case when the buildings are damaged by previous shaking. The degree and distribution of building damages in an urban area is changed as a consequence; see Fig. 16.3 . As 2016 Kumamoto Earthquake clarified, sequential shakings are surely more hostile to structures, and the numerical simulation that considers the effects of past quakes on structural integrity help to estimate the effects quantitatively.

Computational Disaster Mitigation and Reduction Research Unit creates another next generation hazard map for tsunami, using the numerical analysis[1,2] of K computer. The hazard map is fully dynamic rather than static, and provides a video clip which captures tsunami inundation at any site with any viewpoint. Like earthquake, examples of the videoclips are presented in Fig. 16.4 , in which the case that higher and lower seawalls are compared. This next generation hazard map is made with the help of Data Processing Platform, in constructing analysis models of tsunami as well. Two data resources, three-dimensional aerial digital data and two-dimensional Geographic Information System, are used as data resources. Photo-realistic video clips are available for the next generation hazard map, and local government seeks to utilize the map to promote tsunami preparation awareness in resident community.

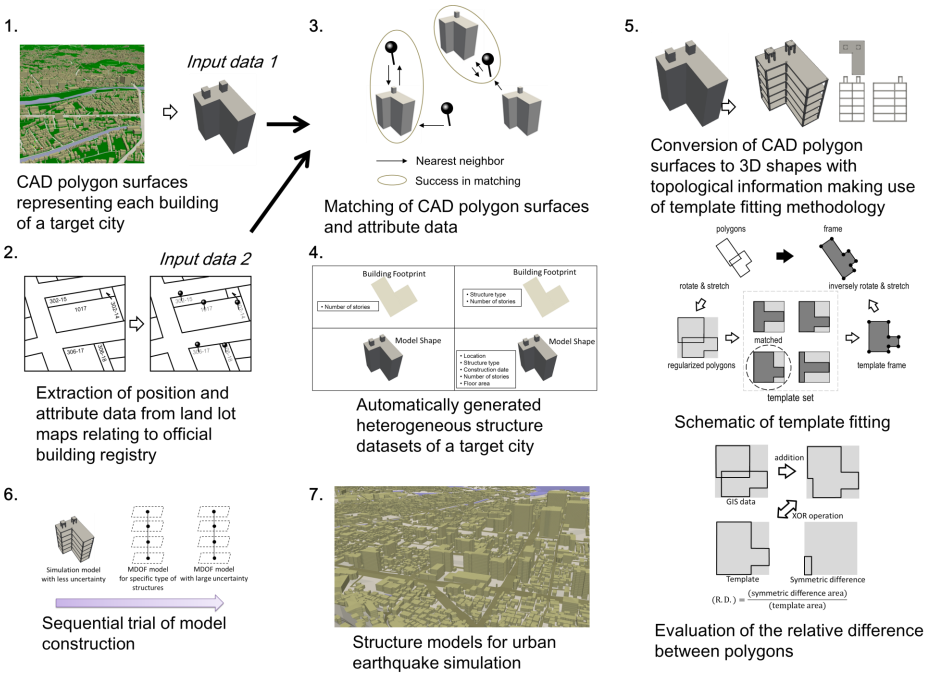

Figure 16.2: Data Processing Platform to generate various urban area models using various data resources

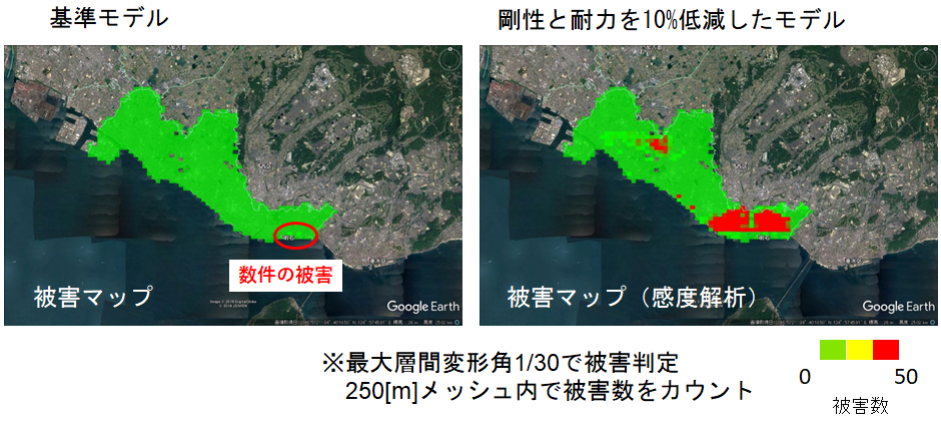

Figure 16.3: Comparison of degree and distribution of earthquake damage of residential buildings by using normal and weak analysis models

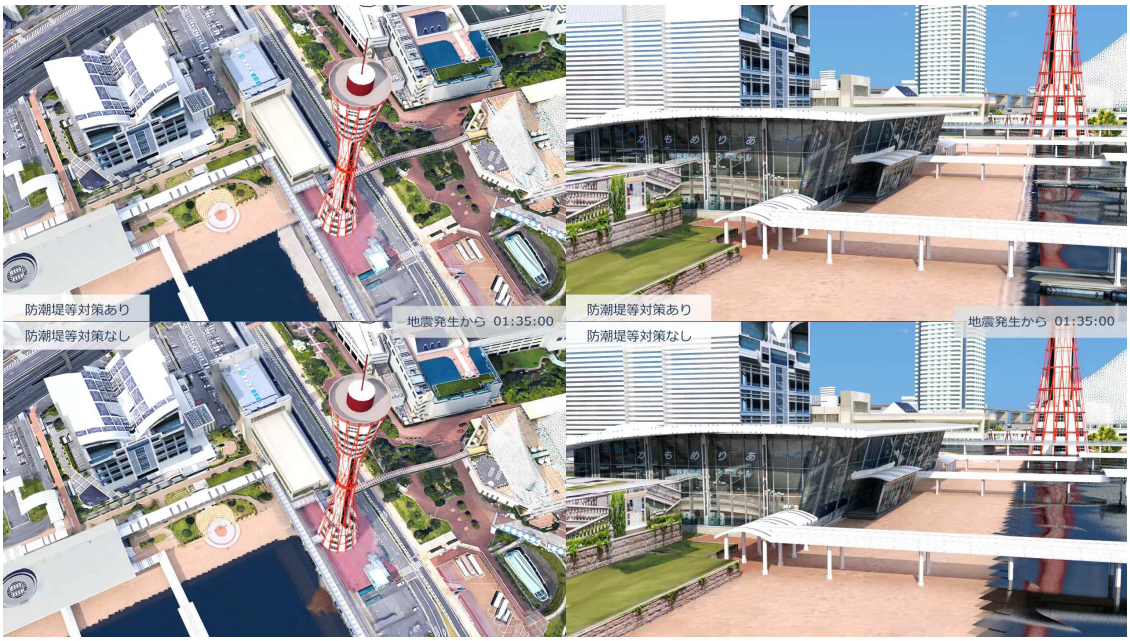

Figure 16.4: Examples of next generation hazard map for tsunami for Kobe City

16.3.2 Development of system for real-time estimate of liquefaction occurrence

Liquefaction is occurred through complicated processes of soil and underground water which are influenced by mechanical properties and permeability of soil and flow of underground water. When underground water pressure increases locally due to the coupling of soil deformation and underground water flow, liquefaction is induced, and it loses ground strength when liquefaction is spread in underground.

Computational Disaster Mitigation and Reduction Research Unit has constructed a system[3-5,11,13-16] that estimates the liquefaction occurrence by using numerical simulation of the above complicated processes of soil and underground water coupling since 2016. The system is now able to make real-time estimate of liquefaction occurrence; for observed ground motion, the system computes 10,000 sites to which analysis models of underground structure are constructed within a few ten minutes, using 1,000 compute node of K computer. A key issue is to improve the performance of numerical analysis method of liquefaction. Figures 16.5 and 16.6 show the speed-up of the method (strong scale) and the break-down of the numerical computation processes. Almost ideal speed-up is observed due to the well tuned numerical analysis processes.

While the numerical analysis method of liquefaction is verified, an analysis model of underground structure which is constructed by using boring hole data is not validated. Material parameters are not fully determined, beside for the applicability of the constitutive relation that is implemented in the analysis method. Uncertainty included in the deterministic numerical analysis ought be estimated; see Fig. 16.7 . To this end, Computational Disaster Mitigation and Reduction Research Unit carries out numerical experiments in which multiple models are constructed for one site or for one boring hole data. The results of the experiment are presented in Fig. 16.8 .

16.3.3 Study on high fidelity model simulation for natural hazard and disaster

High fidelity model simulation is a primary target of capability computing, as it needs a large-scale model and short time to solution. Taking advantage of world top class (or world number one) finite element method[9,10,12,14-16,24-28] enhanced with high performance computing, Computational Disaster Mitigation and Reduction Research Unit studies the following three target: 1) the crust deformation analysis for the prediction of earthquake occurrence processes; 2) the highway network analysis for the estimation of seismic safety against large scale

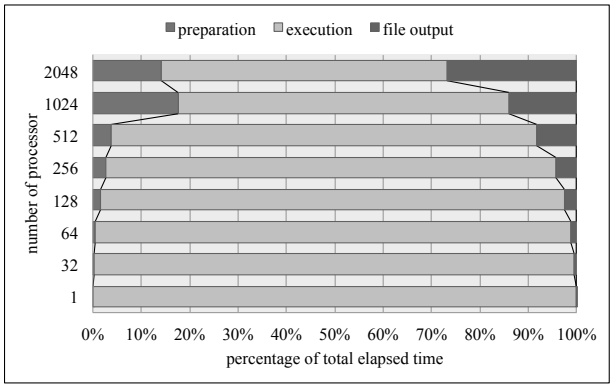

Figure 16.5: Speed-up of the numerical analysis method for liquefaction

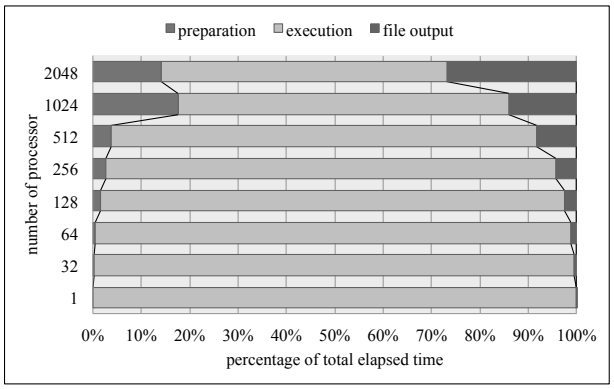

Figure 16.6: Figure 16.6: Break-down of the numerical analysis method for liquefaction

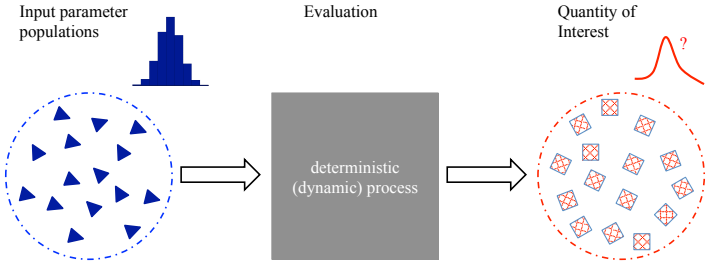

Figure 16.7: Uncertainity estimation for deterministic numerical analysis of liquefaction

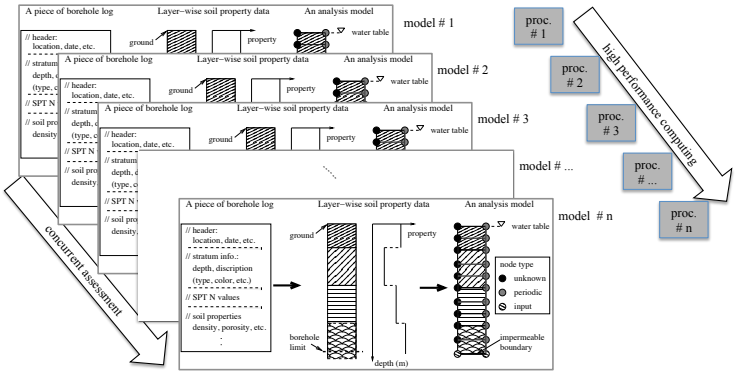

Figure 16.8: Multiple models constructed for numerical experiment of uncertainty estimation of liquefaction

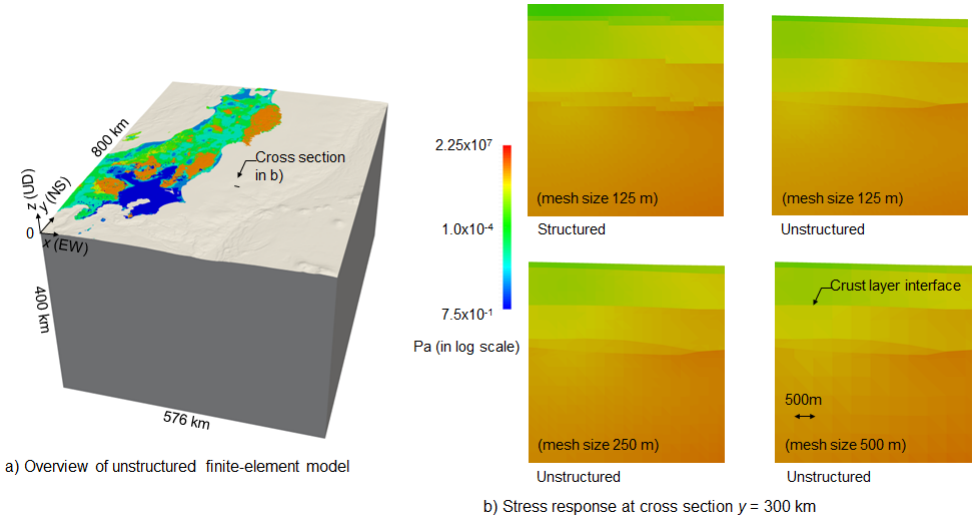

Figure 16.9: Crust deformation analysis

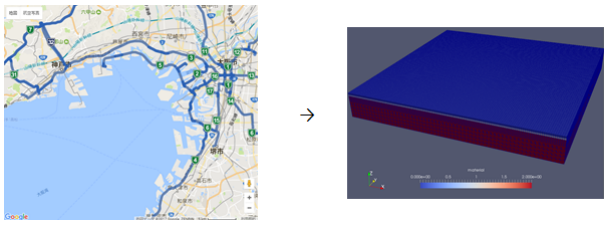

Figure 16.10: High fidelity model of subsurface for highway network seismic response analysis

earthquake[8,21]; and 3) the nuclear power plant building analysis that accounts for non-linear material properties of reinforced concrete[6,16].

The crust deformation analysis uses a large-scale crust model, the construction of which is a challenging subject in the model construction; 10 m resolution is achieved for the inter-plate boundary of complicated configuration. The finite element analysis of this model needs a fast solver, and a pre-conditioner that reduces memory usage drastically is being developed. Figure 16.9 presents the overview of the analysis model and the result of the analysis in which stress accumulation on the inter-plate boundary is computed.

In the collaborative research project with Kobe University and Hanshin Expressway, the unit is constructing a high fidelity model of subsurface (or surface ground layer) in order to compute ground motion distribution which is input to a highway network of a few 10 km or longer; see Fig. 16.10 . While only a small portion (or one span of the network) is studied in ordinary numerical computation, this models enables us to study a more realistic input to the network; the amplitude and phase of the ground motion differ from place to place.

Imitating an international collaborative research project with CAE in France, the unit starts the nuclear power plant building analysis that accounts for non-linear material properties of reinforced concrete. While a multiple mass spring model is often used for a nuclear power plant building for practice, its limitation of evaluating the seismic safety is obvious, especially for large ground motion which induce considerable non-linear responses of local structure components or the overall structure. A high-fidelity model of the building is a more reliable model. The non-linear material properties of concrete or reinforced concrete ought to be accurately computed for such a model; see Fig. 16.11 .

16.4 Schedule and Future Plan

As mentioned, the year of 2016 is the final year of the first phase of the unit. The unit is moving towards more extensive and exclusive research on natural disasters, and the current concern of primary importance is heavy rain in an urban area.

The objectives of the unit research are summarized as follows:

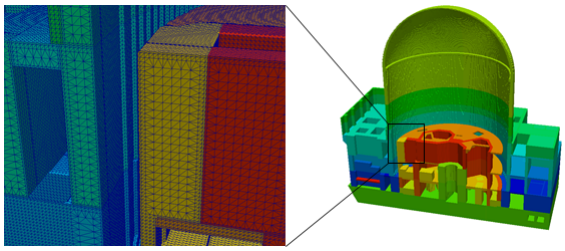

Figure 16.11: Example of a high fidelity model of a nuclear power plant building

Developing Data Processing Platform: Data Processing Platform automatically constructs the urban area models. The development consists of automatic urban model constructer and conceptual representation of components of urban model. These are highly related with Artificial Intelligence research field and Computational Disaster Mitigation and Reduction Research Unit is trying to collaborate with AIP center of RIKEN.

Improving Numerical Analysis Method of Liquefaction: Numerical Analysis Method of Liquefaction will be improved in terms of uncertainty and downscaling. Both of the improvement has been started in 2016, then the improvement will be kept undertaking in the second phase of the unit. Computational Disaster Mitigation and Reduction Research Unit undertake the above two research items with Hanshin Expressway and Kobe University.

Development of Comprehensive Numerical Simulation Method for Natural Disaster: Computational Disaster Mitigation and Reduction Research Unit starts to deal with multiple hazard including geotechnic hazard, flood and sediment related hazard as well as seismic hazard and tsunami hazard. After big earthquake would happen, slope becomes unstable and hazard potential of geotechnic hazard like land slide and mudflow become increase followed by sediment transportation into river bed raising flood risk. Computational Disaster Mitigation and Reduction Research Unit develops comprehensive numerical hazard assessment method consisting of landslide simulation using Smoothed Particle Hydrodynamic Method, hydrological simulation with inundation by shallow water equation and sediment transportation simulation as well as seismic propagation simulation and liquefaction.

Design of Integrated Engineering System (IES): Integrated Engineering System is a platform to assess the risk of natural disaster of all kinds. Risk of natural disaster will take social aspect into account, for example, transportation congestion during evacuation and recovery, risk finance using insurance and reasonable redundancy of lifelines like water supply, sewage water drainage, electric / gas supply and public transportation. By using comprehensive numerical hazard assessment method, Computational Disaster Mitigation and Reduction Research Unit will design the IES with many research partners.

16.5 Publications

16.5.1 Articles

[1] Eguchi, S., Asai, M., O-tani, H., Isshiki, M., "3D Tsunami Run-Up Simulation by Using Particle Method with Geography Analysis Model Including Building Information", Journal of Japan Society of Civil Engineers, A1 (2016)

[2] Isshiki, M., Asai, M., Eguchi, S., O-tani, H., "3D tsunami run-up simulation and visualization using particle method with GIS-based geography model", Journal of Earthquake & Tsunami (2016)

[3] Chen, J., Takeyama T., O-tani, H., Fujita, K., Hori, M., "Using High Performance Computing for Liquefaction Hazard Assessment with Statistical Soil Models", International Journal of Computational Methods (accepted) (2017)

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[5] Supprasert, S., Chen, J.,Maddegedara, L. and Hori, M., "Application of continuumnization and PDS-FEM for the analysis of wave propagation in brick structures", Journal of Japan Society of Civil Engineers, Ser. A2, 72(2) (2016)

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[7] Sahin, A., Sisman, R., Askan, A. and Hori, M., "Development of integrated earthquake simulation system for Istanbul", Earth Planets Space 68 115 (2016)

[8] Hori, M., Wijerathen, L., Ichimura, T., and Tanaka, S., "Meta-Modeling for Constructing Model Consistent with Continuum Mechanics, Journal of Japan Society of Civil Engineers, A2 71(1) I_133-I_142 (2016)

[9] Kohei Fujita, Tsuyoshi Ichimura, "evelopment Of Large-Scale Three-Dimensional Seismic Ground Strain Response Analysis Method and Its Application to Tokyo using Full K Computer, Journal of Earthquake and Tsunami", Journal of Earthquake and Tsunami 10(4) (2016)

[10] Kohei Fujita, Keisuke Katsushima, Tsuyoshi Ichimura, Muneo Hori, Lalith Maddegedara, "Octree-based Multiple-material Parallel Unstructured Mesh Generation Method for Seismic Response Analysis of Soil-Structure Systems", Procedia Computer Science, 80, 1624-1634 (2016)

16.5.2 Conference Papers

[11] Chen, J., O-tani, H., Fujita, K., Hori, M., "High performance computing for liquefaction hazard assessment with statistical soil models", The 7th International Conference on Computational Methods (ICCM2016) 51, 1483-1493 (2016)

[12] Kohei Fujita, Takuma Yamaguchi, Tsuyoshi Ichimura, Muneo Hori, Lalith Maddegedara, "Acceleration of Element-by-Element Kernel in Unstructured Implicit Low-order Finite-element Earthquake Simulation using OpenACC on Pascal GPUs", Proceedings of Third Workshop on Accelerator Programming Using Directives (WACCPD), Best Paper Award (2016)

16.5.3 Posters and Presentations

[13] Chen, J., O-tani, H., Fujita, K., Hori, M., "Application of High Performance Computing for Assessing Hazard of Earthquake induced Liquefaction in Urban Regions", The 2nd Huixian International Forum on Earthquake Engineering for Young Researchers (2016)

[14] Chen, J., O-tani, H., Hori, M., "High Performance Computing for Assessing Hazard of Earthquake induced Liquefaction in Urban Regions", WCCM XII & APCOM VI (2016)

[15] Chen, J., O-tani, H., Hori, M., "Application of High Performance Computing for Liquefaction Assessment Based on Soil Dynamics Analysis", JAEE Annual Meeting (2016)

[16] Hori, M., "Continuumnization of regularly arranged rigid bodies to estimate overall properties", Symposium on The Application of Mechanics to Geophysics (2015)

[17] Hori, M., "Uncertainty and Predictability - Utilization of High Performance Computing for Uncertain Problem", Fukushima Session, Enhancement of Risk-Informed Decision Making against External Natural Events Toward Practical Implementations 2016 ANS Winter Meeting and Nuclear Technology Expo (2016)

[18] Hori, M., "Uncertainty and Predictability - Utilization of High Performance Computing for Uncertain Problem", Expert Meeting on IAEA/ISSC/WA3-2 (2016)

[19] Hori, M., "Earthquake hazard and disaster simulation using urban are model of 10.7x109 degree-of-freedom", Exascale Computing, XXIV ICTAM (2016)

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[22] Hori, M., "Application of High Performance Computing to Earthquake Hazard and Disaster Assessment", 1st International Symposium on Research and Education of Computational Science (RECS) (2016)

[23] Hori, M., "Application of High Performance Computing to Earthquake Hazard and Disaster Assessment", UK- Japan Disaster Research Workshop: Cascading Risk and Uncertainty Assessment of Earthquake Shaking and Tsunami (2016)

[24] Kohei Fujita, Tsuyoshi Ichimura, Kentaro Koyama, Masashi Horikoshi, Hikaru Inoue, Larry Meadows, Seizo Tanaka, Muneo Hori, Maddegedara Lalith, Takane Hori, "A Fast Implicit Solver with Low Memory Footprint and High Scalability for Comprehensive Earthquake Simulation System", SC16 (The International Conference for High Performance Computing, Networking, Storage and Analysis), Best Poster Award (2016)

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[27] Keisuke Katsushima, Kohei Fujita, Tsuyoshi Ichimura, Muneo Hori, Lalith Wijerathne, "Parallel and Robust Tetrahedral Mesh Generation Method for Seismic Response Analysis of Structures", WCCM XII & APCOM VI (The 12th World Congress on Computational Mechanics and 6th Asia-Pacific Congress on Computational Mechanics) (2016)

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Chapter 17

Computational Structural Biology Research Unit

17.1 Members

Florence Tama (Unit Leader)

Miki Nakano (Post-doctoral researcher)

Sandhya Tiwari (Post-doctoral researcher)

Yumeno Kusahara (Assistant)

17.2 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 dynamical 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, ツ providing high-resolution structures. Even though cryo electron microscopy (EM) had provided limited resolution data, it revealed critical information on structure and dynamics of large biological molecules. More recently, efforts like in RIKEN/SPring 8 have focused on developing intense X-ray free-electron laser (XFEL) light sources, which offer a new possibility to image single biological macromolecules. Since crystallization is not necessary for such a protein structure analysis, it would be possible to investigate the structure of biomolecules under various physiological conditions or to observe elementary steps of a biochemical function. However, at the current experimental condition, it cannot achieve atomic level resolution such as obtained by X-ray crystallography. Computationally, methods have been developed to predict structures from low-resolution data such as cryo-EM either using rigid body fitting or flexible deformations of known atomic structures. In addition, even when structures of the molecules are unknown, atomic models can be predicted using homology modeling and ab initio predictions. While ab initio prediction still remains difficult for large proteins, success in predicting small proteins have been observed. Finally, algorithms to analyze protein/proteins interactions also have shown success in predicting proteins complexes.

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

17.3 Research Results and Achievements

17.3.1 Computational tools for XFEL experimental data

Recent development of intense X-ray free-electron laser (XFEL) light sources offers a possibility to obtain new structural information of biological macromolecules. Strong X-ray pulse allows measurement of X-ray diffractions from microcrystals, and furthermore, enables the imaging of single biological macromolecules. Two facilities, SPring-8/SACLA and SLAC/LCLS have been operational in the world and new facilities are becoming available. However, with current experimental conditions, atomic level resolution such as obtained by X-ray crystallography cannot yet be achieved. As XFEL experiments are very recent and still undergoing further development for routine applications to biological molecules, computational algorithms and tools to understand and analyze experimental data also need to be developed simultaneously. One focus of our research is the development of such computational tools from multiple angles summarized below.

"Idea generator" from 2D data of biological systems

Data analysis for XFEL data remains challenging. XFEL diffraction pattern is an unintuitive representation of the projection image of sample in reciprocal space. For biological systems, the current standard approach to reconstruct a real-space image of the sample, phase recovery, often fails due to the low diffraction power of biological samples. Therefore, we are developing a new hybrid approach to interpret diffraction patterns that utilizes image analysis with data mining technique. In this approach, for an obtained XFEL diffraction pattern, the algorithm proposes a few low-resolution 3D models that are consistent with the data using a database of known or hypothetical shapes of biological systems (see Figure 17.1).

To test the feasibility of such approach, we have developed a database of shape, utilizing the existing EM database. We developed a protocol to assemble a non-redundant set of 3D shapes for generating the 2D image library, and tested the retrieval of a potential match. In our strategy, we disregard differences in volume in order to allow for previously unknown structures and conformations that may have a similar shape to be identified. We tested the strategy using images from three EM models as target query images for searches against a library of 22750 2D projection images generated from 250 random EM models. We found that we were able to identify models with shapes similar to the targets, depending on the complexity of the input images and the composition of the search image library (Figure 17.2). This hybrid approach could also be used to estimate the mixing of states or conformations that could exists in such experimental data.

3D structure reconstruction from 2D XFEL diffractions data

Three-dimensional (3D) structural analysis for single particles using X-ray free electron laser (XFEL) enables us to observe hard-to-crystallize biomolecules in a state close to nature. To restore the 3D real structure of the molecule from the diffraction patterns obtained by XFEL experiments, computational algorithms are necessary as one needs to estimate the laser beam incidence angles to the molecule and retrieve the phase information in Fourier space. We are developing a program package for XFEL analysis based on XMIPP, which is commonly used for image processing of single-particle 3D cryo electron microscopy. Since XMIPP is designed to work with 2D data in real space, some of the routine were modified to deal with 2D data in Fourier space. We have reconstructed the structure of a large biological molecule, ribosome, from diffraction data created by computer simulation. A successful estimation of the incident beam angles requires calibration of multiple parameters for image analysis. We have examined such parameters and provided guidelines in their usage to obtain suitable reconstructions. In addition, we have discussed experimental conditions that are required (number of diffraction images, intensity of the laser beam) to restore the molecular structure at a certain resolution. In particular, we were able to demonstrate that structure at 1 nm resolution were achievable for the ribosome given a certain laser beam intensity (see Figure 17.3).

17.3.2 Dynamics at the atomic level by combining X-ray and cryo-EM data

Recent advances in cryo-EM experiments and data processing have produced high-resolution structures of biomolecules. Nevertheless, in many cases, the obtained resolution still remains in the 6-12 テ range, which requires computational techniques to build reliable atomic models. Computational techniques can take advantage of known X-ray structures and use molecular mechanics simulations to optimally deform the structure to match experimental data. In collaboration with the AICS computational biophysics team led by Dr. Sugita, we have been implementing such type of approaches in GENESIS. Taking advantage of the generalized ensemble algorithms embedded in GENESIS to maximize conformational sampling, increase in reliability of the atomic models was achieved. Applications of such methods to experimental data were then performed. More specif-

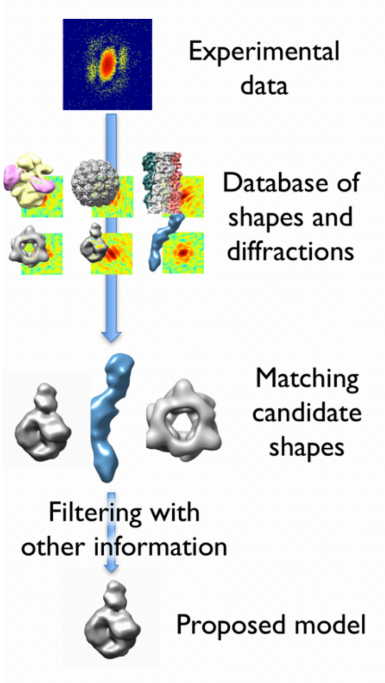


Figure 17.1: Experimental data is given as input. By inquiring database of shapes and corresponding diffraction patterns, candidate low-resolution structural models are proposed.

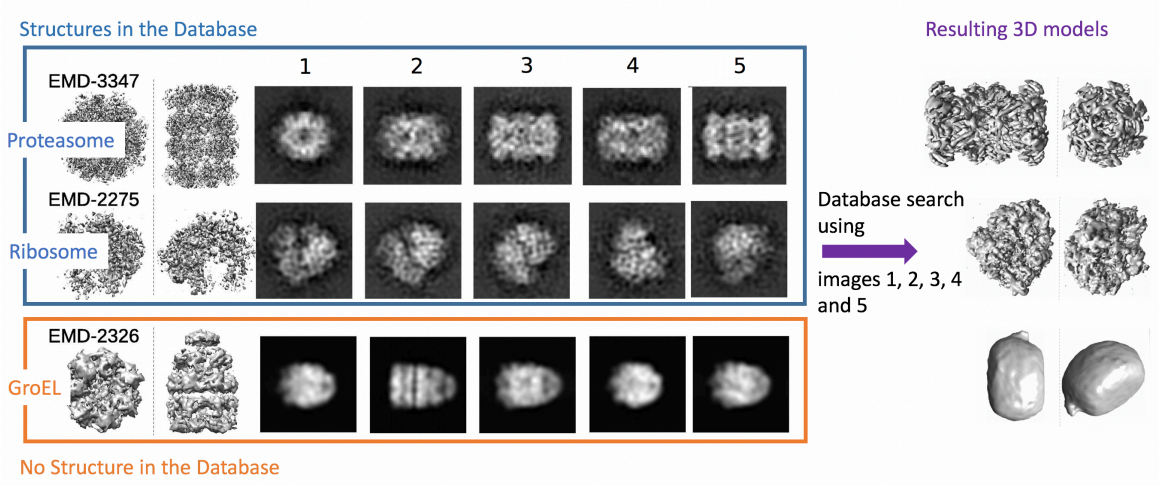
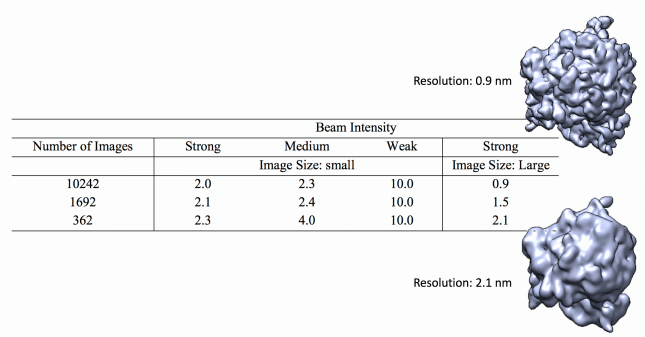


Figure 17.2: Five random 2D projection images used as input for testing 3D initial model search from EMD-3347, EMD-2275 and EMD-2326. Two views of each EM model are displayed below the model name (left) and the input projection images numbered 1 to 5 are displayed in the same row (right). The resulting top search hits is also shown. In the case of EMD-3347 and EMD-2275, we were able to retrieve the most similar 3D models within the first five hits for each. However, the hits for EMD-2326 are less consistent in their shapes and reflect the fact that there is no true match, though the overall shape is consistent to a certain extend.



	Beam Intensity			
Number of Images	Strong	Medium	Weak	Strong
	Image Size: small			Image Size: Large
10242	2.0	2.3	10.0	0.9
1692	2.1	2.4	10.0	1.5
362	2.3	4.0	10.0	2.1

Figure 17.3: 3D reconstruction from XFEL data: resolution of structures using different dataset and bean intensity.

ically, the cryo-EM experimental map of Release Factor 2 (RF2) bound to the ribosome indicates a complex transition with a conformation significantly different from a known X-ray structure of unbound RF2. Therefore, a manual modeling was previously attempted-two domains were moved extensively as rigid bodies to match the EM density. More recent X-ray structures of RF2 bound to ribosome exist, but the conformation of RF2 in these structures do not conform to the map as well as the manually built model. During the fitting process, the correlation coefficient (CC) is used to measure the agreement between the model and the experimental data. Since our approach relies on generalized ensemble algorithms, all structures sampled with a CC over 0.82 can be clustered (1000) to identify potential models. However, overfitting is always an issue for fittings to experimental data, since there is no guarantee that the correct model has the highest CC value. Therefore we may not solely rely on CC values to select the best models and other factors are required to examine the models. To identify over-fitted structures, RMSD values to the initial X-ray structure can be used in addition to the conservation of secondary structures. Structural integrity requires individual RMSD domain to remain low, which was observed for only one of the cluster. Therefore clustering analysis combined with RMSD calculation can be an effective approach to avoid over-fitting models (see Figure 17.4).

17.4 Schedule and Future Plan

Experimental data from cryo-EM and XFEL will continue to grow in numbers and analysis of such big dataset will increase the necessity of high performance computing. We aim to utilize K and post-K to break the limitation of current processing power and to obtain new level of structural information of biological complexes from EM and XFEL data. For this goal, we plan to develop algorithms and software to analyze large dataset to obtain not only structural models as well as dynamical information that can utilize computers in different sizes such as cluster and supercomputer. By sharing the software and results from structural modeling with other research institutes, we aim to contribute to the structural biology community.

XFEL facility SACLA started its operation in 2012 and applications to biological samples are now providing results. The number is still limited, but data for systems, such as viruses and organelles, are being obtained. The approaches we have developed can predict structural models from a few images. However, with the advancement of experimental techniques, more than 10,000 XFEL diffraction images could be soon obtained, and furthermore, theoretical studies suggest that 1 million images are necessary to obtain high resolution models. In the near future, we will need to utilize such large amount of dataset to reconstruct detailed 3D models from XFEL data. Thus, we will be exploring methods to efficiently construct 3D models from XFEL diffraction patterns. We have produced a framework for such reconstruction and applications with experimental data will soon be started. Additional research is required to establish the software tools for more general applications. These programs need to be improved further to allow the analysis of anticipated large dataset, utilizing HPC.

From these projects, new techniques for data analysis will become available, which will provide new structural information on biomolecules. Using the developed programs, we will work with experimental groups to obtain revolutionary structural information and contribute to the understanding of mechanism of biological functions. We will maintain the new software and also provide usage support so that it is easily accessible to experimental groups from other institutions.

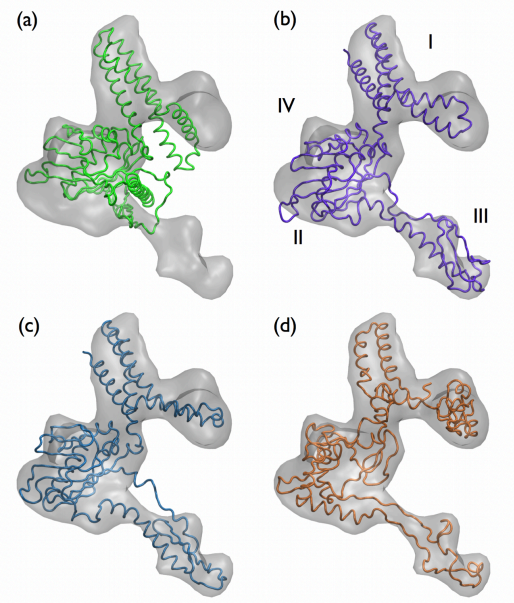


Figure 17.4: a) X-ray structure of unbound RF2 aligned to RF2 experimental data. b) A model created by rearranging the domains as rigid bodies to fit the map. c) A proposed high quality model of RF2 fitted into the experimental data which has the lowest domain deformations from initial X-ray structure. d) A low quality model with the highest CC value. While it has high CC value, many secondary structures are not preserved.

17.5 Publications

[1] Three-dimensional reconstruction for coherent diffraction patterns obtained by XFEL. M. Nakano, O. Miyashita, S. Jonic, C. Song, D. Nam, Y. Joti and F. Tama. J. Synchrotron Rad. 2017

[2] Flexible Fitting to Cryo-EM Density Map using Ensemble Molecular Dynamics Simulations. O. Miyashita, C. Kobayashi, T. Mori, Y. Sugita, F. Tama. J. Comp. Chem. 2017

[3] Editorial overview: Macromolecular assemblies. T. Shimizu and F. Tama. Curr. Opin. Struc. Biol. 2017

[4] Hybrid approach for biological structure modeling: cryo-electron microscopy and X-ray free electron laser data. O. Miyashita and F. Tama. Seibutsu Butsuri 2017 (in Japanese)

Part II

Operations and Computer Technologies Division

Operation status and research activities of Operations and Computer Technologies Division are presented in this part. Operation and Computer Technologies Division are responsible for operation and enhancement of the K computer and the facilities. Operation and support of High Performance Computing Infrastructure (HPCI) system are also a part of our missions. Our division consists of four teams. The missions and members of the teams are shown as follows:

- Facility Operations and Development Team (Team Head: Toshiyuki Tsukamoto)
  Missions: Operation and Enhancement of the facility for the K computer
  Members: Technical Staff(6)

- System Operations and Development Team (Team Head: Atsuya Uno)
  Missions: Operation and Enhancement of the K computer
  Members: R&D Scientist(5), Technical Staff(2)

- Software Development Team (Team Head: Kazuo Minami)
  Missions: Operation and Enhancement of the K computer software and application tunning
  Members: R&D Scientist(6)

- HPCI System Development Team (Team Head: Manabu Hirakawa)
  Missions: Operation and Enhancement of HPCI system and logistics of the HPCI activity
  Members: R&D Scientist(1), Senior Visiting Scientist(2), Visiting Scientist(1)

Four and a half years have passed since the start of the K computer official operation. (Actually six years have also passed since the start of early access which was a service for limited user.) Needless to say, it is important to reduce the irregular system down time for stable service. To realize it, we continue to investigate the causes of failures and develop workarounds to reduce the impact of such a system failures. Actually, we could achieved lower irregular service down time than that of JFY2015 which corresponse to only 4.56 days per a year. We also tried to improve energy efficiency of the faicility and system usability, etc. The detail of the operational improvements and research activities are also reported in the following chapters. We hope readers find our experences and lessons learned informative.

Chapter 18

Facility Operations and Development Team

18.1 Members

Toshiyuki Tsukamoto (Team Head)

Mitsuru Tanaka (Technical Staff)

Hiroyuki Takitsuka (Technical Staff)

Satoru Matsushita (Technical Staff)

Katsuyuki Tanaka (Technical Staff)

Humio Tsuda (Technical Staff)

Hiromi Matsuki (Technical Staff)

Hajime Naemura (Technical Staff)

18.2 Research Activities

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

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

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

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

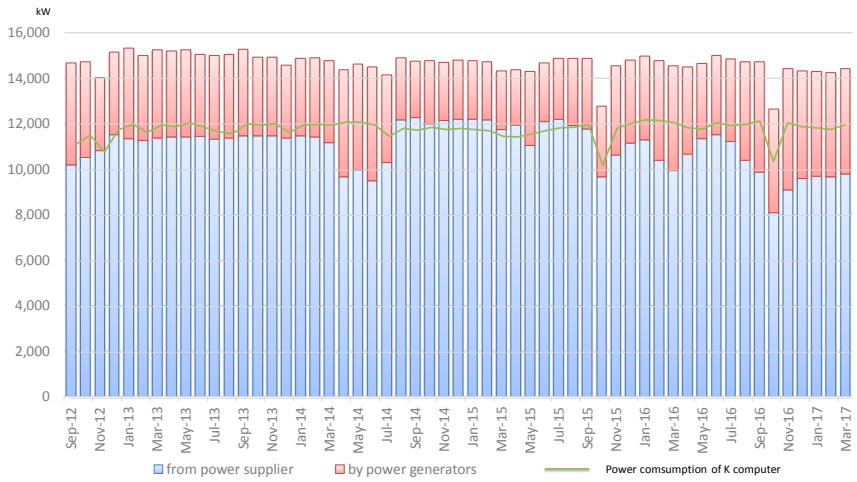


Figure 1: Monthly power supply and K computer power consumption

18.3 Research Results and Achievements

18.3.1 Optimum operation of electric power

Figure 1 shows the monthly total power supply and the power consumption of K computer from September 2012 to March 2017. The status of power supply, which consists of commercial power purchased from a supply company and the power generated by CGS.

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

As shown in Figure 1, AICS' electric power supply consists of commercial and CGS power. There are two CGS systems in AICS, and they are used by turn for two weeks at a time. Therefore, at least one CGS is always in use. Commercial electric power is covenanted at about 12,500 kW, and power consumption was approximately 12,000 kW (annual average), which corresponds to approximately 90% load factor.

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

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

18.3.2 Improvements to power usage effectiveness (PUE)

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

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

Figure 2 indicates a change in the annual average power consumption of K computer (including the peripheral devices) and cooling equipment. After FY2013, the power consumption of K computer has been almost flat at approximately 11,800 kW, but the power consumption of the equipment decreased gradually from FY2013 to FY2016. Accordingly, the PUE of AICS improved to 1.324 in FY2016 from 1.447 in FY2012, thus contributing to reduction in electricity cost.

In FY2013, we reduced the electricity cost of air-conditioners by reducing the number of working air-conditioners. Total cooling performance was maintained by lowering the air temperature. We could achieve a reduction of 217 kW in power consumption.

In FY2014, we focused on the fault-tolerance feature of the air-conditioning equipment. Each air-conditioner has two motors for fault-tolerance. We found that if one of the two motors could be stopped, airflow could be maintained at approximately 60%. Thus, we reduced power consumption by a further 277 kW in FY2014, and by 24 kW in FY2015.

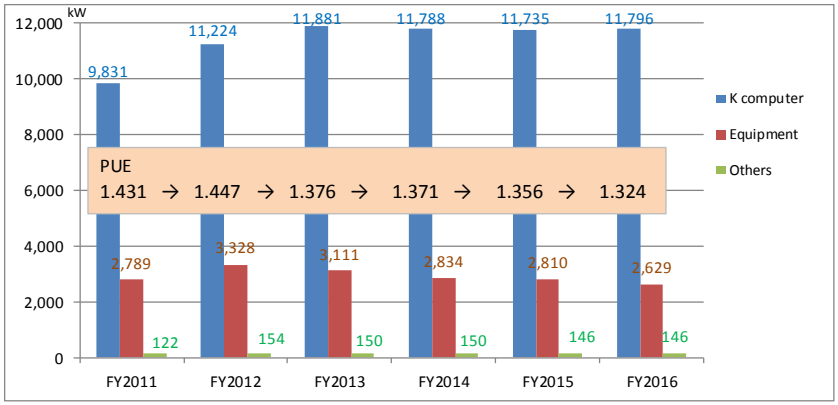


Figure 2: Trend in annual average electric power consumption

In FY2016, we worked on improving the efficiency of the cooling tower. As a result, we could achieve a reduction of 181 kW in power consumption.

18.4 Schedule and Future Plan

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

18.5 Publications

18.5.1 Journal Papers

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

[2] Keiji Yamamoto, Atsuya Uno, Hitoshi Murai, Toshiyuki Tsukamoto, Fumiyoshi Shoji, Shuji Matsui, Ryuichi Sek-izawa, Fumichika Sueyasu, Hiroshi Uchiyama, Mitsuo Okamoto, Nobuo Ohgushi, Katsutoshi Takashina, Daisuke Wakabayashi, Yuki Taguchi, and Mitsuo Yokokawa. The K computer operations: Experiences and statistics. In Proceedings of the International Conference on Computational Science, ICCS 2014, Cairns, Queensland, Australia, 10-12 June, 2014, pages 576-585, 2014.

[[3] Fumiyoshi Shoji, Shuji Matsui, Mitsuo Okamoto, Fumichika Sueyasu, Toshiyuki Tsukamoto, Atsuya Uno, and Keiji Yamamoto. Long term failure analysis of 10 peta-scale supercomputer. In HPC in Asia session at ISC2015, Frankfurt, Germany, July 12-16, 2015.

18.5.2 Conference Papers

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

[5] Lili Jin, Kouji Yutani, Hiroyuki Yamano, Hiroyuki Takitsuka, Satoshi Matsusita, Toshiyuki Tsukamoto, 計算科学研究機構における設備最適運転条 件の検討その２, Proceedings of the 49th Japanese Joint Conference on Air-conditioning and Refrigeration(Tokyo). (In Japanese)

[6] Satoshi Matsushita, Hiroyuki Takitsuka, Toshiyuki Tsukamoto, スーパー コンピュータ施設における低騒音空調機の省エネ運用, Proceedings of the 49th Japanese Joint Conference on Air-conditioning and Refrigeration(Tokyo). (In Japanese)

18.5.3 Posters and Presentations

[7] Fumio Inoue, Atsuya Uno, Toshiyuki Tsukamoto, Satoshi Matsushita, Fumichika Sueyasu, Naoki Ikeda, Hajime Hida, Fumiyoshi Shoji, 電力消費量の 上限を考慮した「京」の運用, IPSJ-SIGHPC 2014-HPC-146 No.4, 2014. (In Japanese)

[8] Atsuya Uno, Hajime Hida, Naoki Ikeda, Fumio Inoue, Toshiyuki Tsukamoto, Fumichika Sueyasu, Fumiyoshi Shoji,「京」におけるジョブ単位の消費電力推定 の検討, IPSJ-SIGHPC 2014-HPC-147 No.20, 2014. (In Japanese)

Chapter 19

System Operations and Development Team

19.1 Members

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19.2 Research Activities

K computer, a distributed-memory parallel computer comprising 82,944 computing nodes, has played a central role in the High Performance Computing Infrastructure (HPCI) initiative granted by the Ministry of Education, Culture, Sports, Science and Technology. The HPCI has achieved the integrated operation of the K computer and other supercomputer centers in Japan. Further, it has enabled seamless access from user machines to a cluster of supercomputers that includes the K computer. Moreover, the HPCI has provided large-scale storage systems that are accessible from all over Japan.

The system operations and development team (SODT) has conducted research and development on the advanced management and operations of the K computer. While analyzing operational statistics collected during shared use, the SODT has improved the system configuration, including aspects involving job scheduling, the file system, and user environments.

In the fiscal year 2016 (FY2016), we primarily implemented improvements to the following operational issues:

- Improvement of waiting time for jobs
- Response degradation problem of the global file system
- Appropriate disk utilization toward effective job scheduling
- Monitoring I/O performance of jobs
- Considering the introduction of long-term jobs
- Optimization of maintenance operations
- Estimation of electric power of jobs

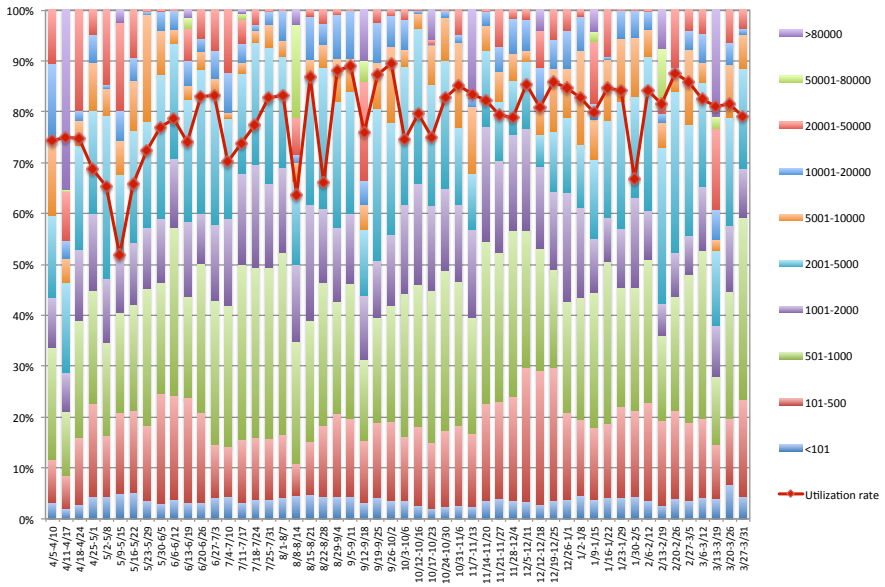


Figure 1: Resource usage in FY2016

19.3 Research Results and Achievements

Figure 1 shows resource usage details for FY2016. As depicts in the figure, we achieved approximately 79% utilization rate, which is greater than that achieved in FY2015 (75%). The improvement of utilization in April and the optimum use of low-priority service are the reasons why the utilization rate was higher than last year. The utilization rate in April each year was 50%–70%. However, in FY2016, it was 70%–80% during the same period. With the low-priority service that was introduced in FY2015, jobs can be executed with low priority even in projects where allocated resources have exhausted. In comparison to FY2015, when users used 1.8 million node hours, in FY2016, users used 9.7 million node hours. These led to the improvement in the utilization rate.

19.3.1 Analysis and improvement of operational issues

19.3.1.1 Improvement of waiting time for jobs

Figure 2 shows the average waiting time of large jobs (i.e., 12289–36864 nodes) without low-priority jobs in both FY2015 and FY2016. Compared with FY2015, the waiting time in FY2016 has become very short. In FY2015, as a method to shorten the waiting time, we changed the region used by higher priority jobs to a region that may not inhibit the execution of normal priority jobs. In FY2016, we improved the scheme of priority control in job scheduling. In the previous scheme, normal priority jobs could not overtake higher priority jobs no matter how long they waited. In FY2016, when the waiting time becomes long, the normal priority job was executed even if there were higher priority jobs. Therefore, the waiting time for normal priority jobs were kept shorter, leading to a significant improvement in throughput of job execution.

19.3.1.2 Response degradation problem of the global file system

A temporary response reduction of the global file system (GFS) has occurred several times. A major factor is the load concentration to the GFS due to large-scale file staging. Since the bandwidth of the storage is occupied by the file staging, there is a big I/O interference in other light weight file accesses.

We analyzed the scheduling of the jobs and found the following two factors had an impact on the long waiting time.

- Automatic striping of stage-out file
- Fair-share I/O thread allocation setup for accesses from frontend servers and file staging

We have already adopted the first optimization by taking the file size into account to choose the appropriate stripe count in the stage-out phase, and this approach has achieved a better situation to mitigate response degradation. For further improvements, we have addressed better ways for stripe count optimization. Besides,

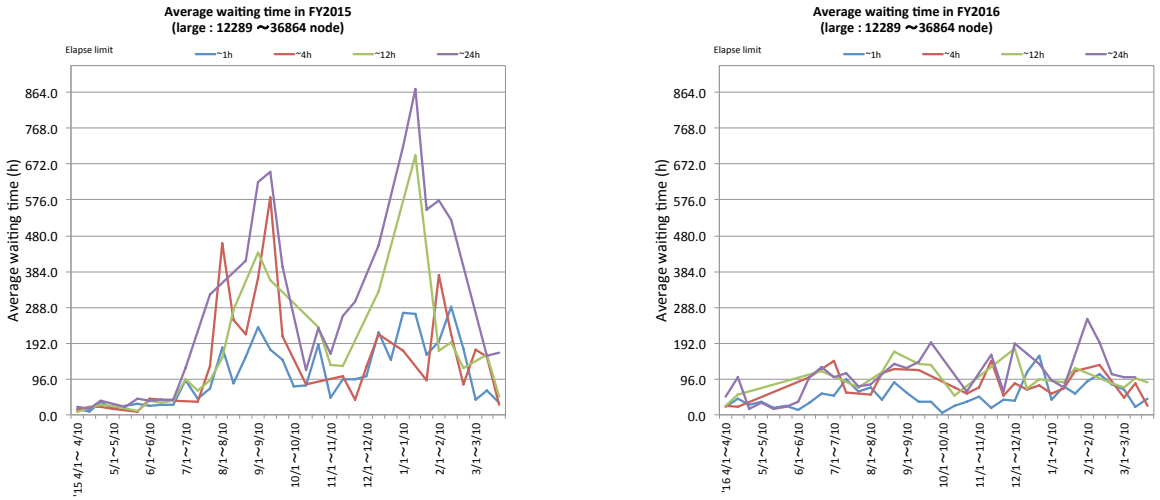


Figure 2: Average waiting time in FY2015 and FY2016

a quality of service (QoS) function of Fujitsu Exabyte File System (FEFS) has been incorporated, where FEFS is a parallel file system used at the K computer based on Lustre technology. The QoS supports fair-share I/O workload by limiting the number of service threads on Object Storage Server (OSS) or Meta Data Server (MDS) of the FEFS file system among clients or users.

We model stripe count optimization in the first approach. In general, as the larger stripe count increases, the better I/O workload of Object Storage Target (OST) of the GFS is evenly distributed in striping accesses of parallel file systems. Conversely, we may have a sort of increases in I/O accesses times due to overestimated stripe count. In this context, we have addressed to find the minimum optimal stripe count that leads to a balanced I/O workload among OSTs.

Here, we consider the stripe count optimization model in stage-out operations through our examinations of both the theoretical and experimental performances. The second optimization using the QoS function of FEFS addresses to have fair-share I/O workload at OSSs of the GFS for each client group. For instance, we can split clients in several groups by the source IP address. In our file staging scheme, the introduced QoS has realized a balanced situation among I/O streams from frontend and Global I/O (GIO) nodes in the stage-out phase.

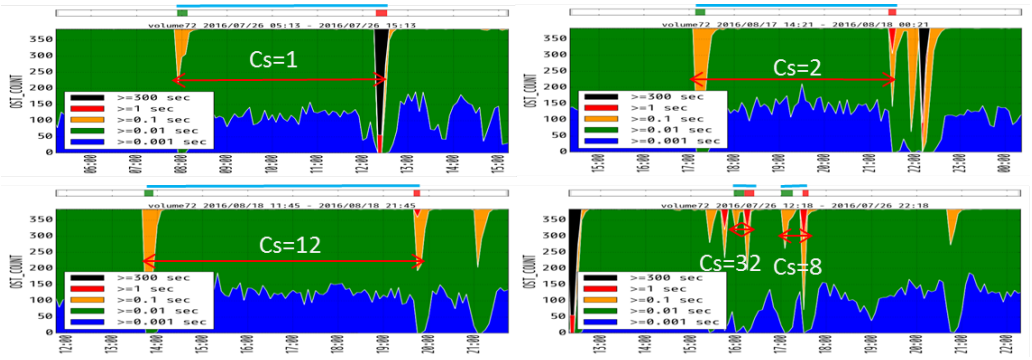
The above two optimizations were evaluated to study their effectiveness for the K computer using one GFS volume comprising 384 OSTs, which was apart from the normal job operation to eliminate interference by other user applications.

Figure 1 depicts response times in 1 MiB write for 384 OST each by `dd` from a frontend node while huge file staging of 576 files, 12 GiB each, was performed using 96 GIOs in terms of the stripe count (C_S). The upper four graphs in Fig. 1(a) depict response times with only stripe count optimization, where we chose five patterns (1, 2, 8, 12, and 32) for C_S. The vertical axis denotes the number of OSTs, and the response time distribution among 384 OSTs is depicted in five colors over 10 hours along the horizontal axis. A big degradation is observed for the stage-out phase with a single stripe count (C_S=1). An increase in the stripe count leads to mitigation of response times, and we have found 12 in the stripe count was the best. It is also remarked that 14 in the stripe count is the best case in our stripe count optimization model if we accept up to 5% variance of I/O workload among OSTs. We have confirmed the effectiveness of the performance model under several configurations, although we have not described all results in detail due to the limited space of this report.

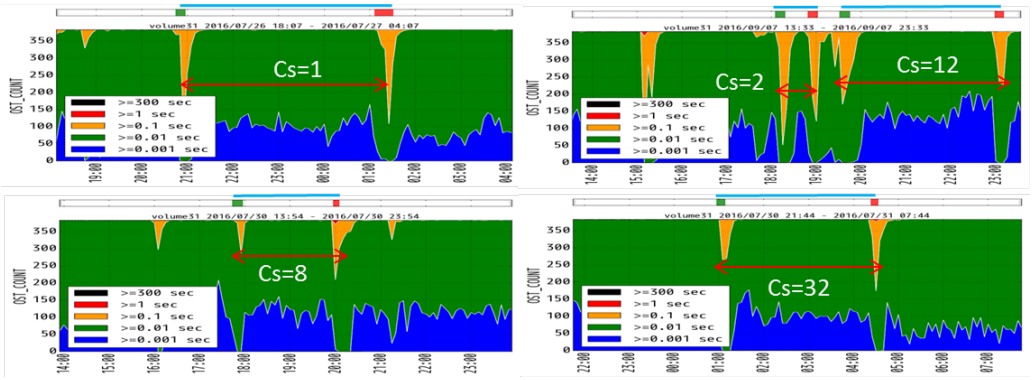
An improvement in response time was observed by adopting the QoS function of FEFS in parallel with the stripe count optimization, as shown in the lower four graphs of Fig. 1(b). Even during a single stripe count stage-out operation, response time was improved by the QoS adoption compared with Fig. 1(a). In this example, we found that the 12 stripe count with the QoS function of FEFS was the best case. The optimizations described here are still in progress, and we continue to find a better optimization than we have.

19.3.1.3 Appropriate disk utilization toward effective job scheduling

The amount of available disk space of each compute node can be changed by using a parameter named “node quota” in job scripts, when users require larger space for their file I/O. However, there might be a delay in job scheduling including file staging to secure enough disk space. Such delay in job scheduling not only occurs in



(a) Only stripe count optimization



(b) Both stripe count and QoS optimization

Figure 3: Response times of write operations by `dd` from frontend nodes during huge file staging of 576 files, 12 GiB each, by 96 GIOs, where C_S represents stripe count.

jobs with overestimated node quota but also in other jobs. From our operation experience, some users have specified an overestimated size of the node quota due to misunderstanding of this option. Through K computer operation, we have been observing differences between the node quota value and actual disk usage. Further, we have been periodically asking users utilizing extremely overestimated node quota to correct the appropriate value. Through this approach, we have observed improvements in job scheduling efficiency compared with the last fiscal year.

19.3.1.4 Monitoring I/O performance of jobs

In FY2015, we started collecting performance data regarding the GFS and local file system (LFS) to monitor load. We used these data to detect failures and to analyze the I/O performance of each job. In FY2016, we have collected a number of metadata operations such as open, close, and getattr, per job. These metadata operations are executed on metadata server (MDS). We can identify jobs that put a heavy load on the file system. Depending on the state of the file system, a mechanism to detect high-load jobs was implemented.

Figure 4 shows the number of metadata operations, such as open, close, and getattr, on LFS. This graph shows the local MDS (LMDS) performance on LFS. This graph is updated every minute. The left and right graphs depict the the number of total operations and the number of operations per job, respectively.

19.3.1.5 Consideration to introduce long-term job

Since some users requested job execution exceeding 24 hours, we considered the introduction of long-term jobs. We investigated the influence on waiting time for normal jobs and the influence of node failure by introducing long-term jobs up to 72 hours. As a result of the examination, long-term jobs will be introduced from FY2017.

19.3.1.6 Optimization of maintenance operations

In a massive parallel system, even if the failure rate per node is low, reduction of the failure rate is difficult in the case of entire system. By performing repairs every time a fault occurs, minimizing the influence of the fault

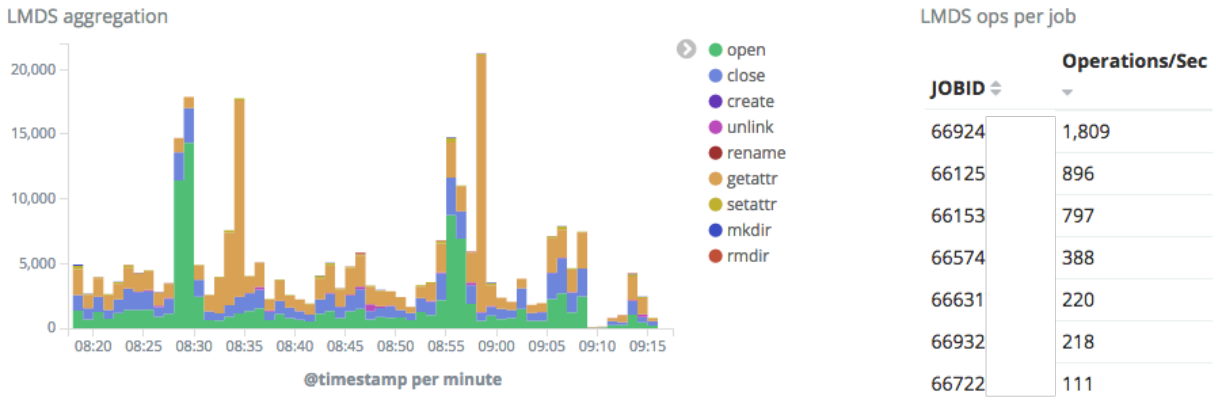


Figure 4: Number of metadata operations on LFS

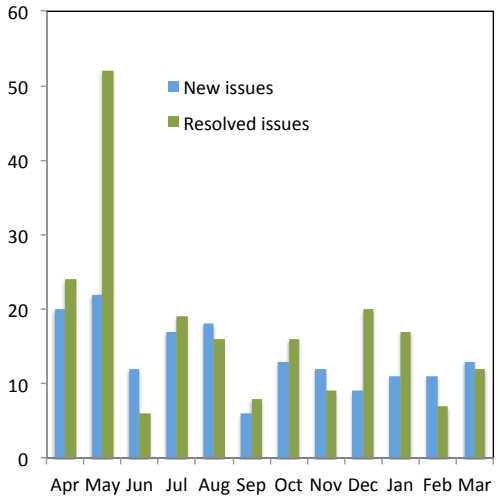


Figure 5: Number of issues addressed in FY2016

on the operation is possible. However, maintaining such a system repairing is difficult from the aspect of the cost. Therefore, we examined the relation between node failure and operation efficiency. We found that the number of maintenance can be reduced without lowering the operation efficiency.

19.3.1.7 Power consumption prediction

From FY2015, we have tackled prediction of power consumption of the jobs. The power consumption for each job being executed is estimated based on the thermal sensor of the compute rack. We created a new thermal model from the physical configuration of the system board. We predicted the power consumption and improved the predicted error to about 2%. This is the result of collaborative research with Fujitsu Laboratories.

19.3.2 User support

The K computer had approximately 190 projects in FY2016. The number of active daily users was approximately 120.

We supported users through the K support desk and provided users with technical information regarding the K computer, including information regarding its system environment, system tools, and software libraries. In addition, we performed user registrations, failures investigation, software installation, etc. We offered our consulting services together with the software development team. Figure 5 presents the number of issues addressed in FY2016, showing the number of new issues in FY2016 to be approximately 160; the number of resolved issues was approximately 210. The number of new issues in FY2015 was approximately 230.

19.4 Schedule and Future Plan

In FY2016, we primarily performed improvements on operational issues. Analyzing various logs and metrics from the system leads to early detection of the problem. To tackle a detected problem before it becomes a serious problem, we plan to continue the analyses in FY2017. Moreover, we continued trying to improve the user environment and provide user support.

19.5 Publications

19.5.1 Posters and Presentations

[1] Atsuya Uno, "Operation Experiences of the K computer", SIAM Conference on Parallel Processing for Scientific Computing, 2016

[2] Yuichi Tsujita, "Understanding and Improving Storage Accesses at the K computer", Understanding I/O Performance Behavior Workshop, 2017

Chapter 20

Software Development Team

20.1 Members

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20.2 Research Activities

Collaboration between the K computer system and its applications is key technology for creating innovative results. In order to maximize application performance, system reliability, and usability, the Software Development Team has been conducting the following activities: (1) efforts have been made to maintain stable operation of the K computer and to provide support for users to obtain innovative outcome, (2) research have been conducted to obtain high-level operational efficiency of the K computer, and (3) research have been performed to improve application performances.

20.3 Research Results and Achievements

20.3.1 Operations of the K Computer

20.3.1.1 User Support

We offer K support desk service to users in collaboration with the system operations and development team. The K support desk's role is to solve any queries from users, which are raised by both RIKEN AICS users and general users indirectly via the Research Organization for Information Science and Technology (RIST). RIST is an official organization that is engaged in consultation services for K computer general users. We are in charge of compilers, profilers, programming support tools, debuggers, numerical libraries, a Message Passing Interface (MPI) library, user manuals, and tutorial documents.

The K support desk addressed 688 technical enquiries, requests, and problem reports in FY2016. Weekly meetings are held by the staff of the K support desk to monitor the progress toward solving these issues.

20.3.1.2 Study on Runtime Fluctuations

Runtime fluctuations are differences in the runtime of an application, which occur despite the application being run under the same execution conditions and manner. These fluctuations disturb the efficient operations of the K computer. Therefore, runtime fluctuations need to be studied and resolved.

Previously, we encountered and solved some causes of runtime fluctuations, including (1) jitters caused by an asynchronous I/O that is the basic function of a modern OS, (2) access concentration to a load module file caused by numerous processes in a huge scale parallel job, (3) increasing number of operations due to software-based processing for the de-normalized numbers that defined in IEEE754 floating point arithmetic, (4) changing a state of cache thrashing derived by the address space layout randomization that is one of the basic security functions of a modern OS, (5) translation lookaside buffer (TLB) thrashing caused by the shortage of large page size, and (6) degradation of performance due to increasing cost of frequent operations of large page, i.e., allocation, initialization, and deallocation. Our efforts to address the problems caused by runtime fluctuations were reported in a paper and some conferences [3][11][12][13].

20.3.1.3 Checking the System Performance

When the system software, including operating systems, compilers, and libraries, are updated, we need to check if the update has any side effects on the execution of some applications. Therefore, we regularly test the performance using the check suite, a tool to check the comprehensive system performance. In FY2016, three consecutive updates of the language environments, which included the compilers and the libraries, K-1.2.0-20, K-1.2.0-21, and K-1.2.0-22, were released, and each environment was checked. According to the result of the check suite, we detected a few performance degradations. Results of the investigation ascertained that the language environments were not the cause of performance degradation. As a result, all language environments were formally released to all users.

1. K-1.2.0-20: 3 cases of degradation (QCD, Seism3D)

2. K-1.2.0-21: 5 cases of degradation (FFB, NICAM, Seism3D)

3. K-1.2.0-22: 3 cases of degradation (NICAM)

20.3.1.4 Release of MPI Performance Data

In FY2016, we evaluated the validity of the performance of major communication functions of the MPI library; it was already measured in FY2014. A communication performance can be evaluated by two parameters: one is bandwidth, which is dominant in long message size, and the other is latency, which is dominant in short message size. The measured values of bandwidth and latency can be calculated from the peak performance and the half-performance length. The half-performance length is the message size at which the measured communication throughput is half of the maximum. The estimation formula of the communication time can be derived theoretically from the model of communication behavior. We compared the estimated bandwidth and latency with the measured values in a wide range of message sizes. There were differences between the estimated and the measured. The differences were up to about 20% in peak performance and up to about 50% in latency. However, the measurement results showed the same trend as estimation results [1][5].

20.3.2 Development of Tools

20.3.2.1 K-scope: The Fortran and C Source Code Analysis Tool

K-scope is a Fortran and C source code analysis tool that uses intermediate codes exported by the front-end of the Omni compiler. To find bottlenecks (e.g., multiple nested loops) from source codes, performance engineers can use K-scope before rewriting source codes to improve performance. Since FY2012, we have been distributing K-scope as part of the AICS software. Furthermore, in collaboration with Kobe University in Japan, we developed the Eclipse plugin to visualize the Fortran source code structure on the framework and distributed the source codes via GitHub [17][20].

20.3.2.2 New Hardware Counter Tool on the K Computer

In FY2015, we investigated the hardware counter of the K computer and examined the improvement of the analysis tool of the hardware counter. The improved tool was registered as AICS software "1PAtool" and installed on the K computer [21].

In FY2016, we changed the method of reporting. Old tool reported the counter value of each process. New tool reports the counter value of an application.

20.3.3 Improvement of the Operational Efficiency

20.3.3.1 Introduction

Recently, various problems have been reported in operations of the HPC system. The fluctuations of job execution times are one of the difficult problems that need to be investigated and solved as they cause complications. There are cases wherein the fluctuation of execution time is large. In such cases, jobs are not completed within their scheduled time. As a result of the analysis, it was found that there were cases wherein loads of metadata servers on the local I/O (LMDS) were saturated due to achieving its performance limit. In FY2016, we focused on I/O performance and analyzed the load of LMDS instructions by jobs.

20.3.3.2 Analysis of Local MDS Load

In FY2015, we constructed the job performance database on the job analysis server [6][14][15][16]. In FY2016, the number of LMDS instructions of each job I/O was added to the database. We analyzed the LMDS loads due to job I/O using this database [7].

Figure 20.1 shows the transition time of the number of LMDS instructions during a period. In this figure, there are three heavy jobs for LMDS. It also contains the total and other jobs, excluding the three heavy jobs. This figure shows that when job1 exceeded 25,000 [OPS], job2 and job3 could not access LMDS because of saturation.

The number of MPI processes of jobs having a high load for LMDS mentioned above was about 2,000, which was not so large. The jobs having a high load for LMDS often use the shared files instead of the local files on the local I/O file system, and then the number of LMDS instructions tends to increase in proportion to the number of MPI processes. Therefore, we investigated the number of MPI processes at which the load of LMDS instructions saturates. The number of the saturated MPI processes was calculated as follows: (1) Each job has its own number of LMDS instructions A and number of processes B. (2) The saturated MPI process is defined as $25,000 \div A \times B$.

In Figure 20.2, the blue line indicates the histogram of the saturated MPI processes. From this figure, it can be observed that the number of jobs increases rapidly in the range from 300 to 1000 MPI processes. It was found that the load of LMDS was saturated easily even if the number of the MPI processes was small.

In Figure 20.3, there are three values. The blue line indicates the number of jobs that saturate the load of the LMDS (called saturating job), the red line indicates the length of the time when the load of LMDS is saturated (called saturated time), and the green line indicates the wasted node hour when the number of MPI process is increased until it gets doubled. Figure 20.3 illustrates that if the number of MPI process is doubled, the number of saturating jobs is increased by 6 times, the saturated time is increased by 14 times, and therefore the wasted node hour is increased by 28 times. It is predicted that the load saturation of the LMDS will occur more frequently with a significant increase of processes in the future. It is, therefore, important to monitor the load of the LMDS through jobs using shared files.

20.3.4 Research and Development of Techniques to Improve the Computational Performance of Application Programs

20.3.4.1 High Performance Conjugate Gradient (HPCG) Performance Improvement on the K Computer

The HPCG benchmark program has been proposed as one of the realistic performance metrics for supercomputers. HPCG measures the speed of solving symmetric sparse linear system equations using the frequently used conjugate gradient method preconditioned by a multigrid symmetric Gauss-Seidel smoother.

We evaluated and improved the performance of HPCG on the K computer using the early version before its official announcement. HPCG showed good parallel scalability; however, its single CPU performance was very low.

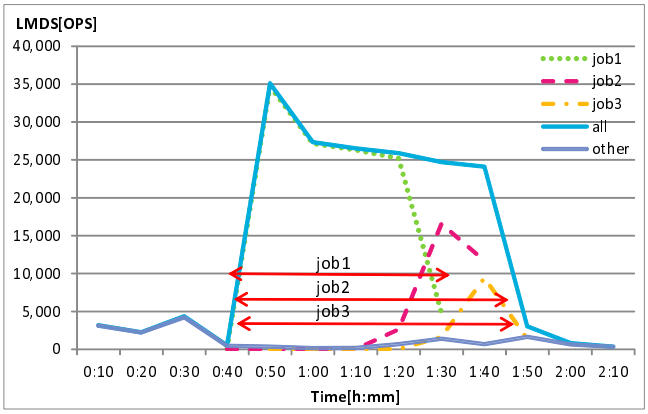


Figure 20.1: Impact of occupation of LMDS by job

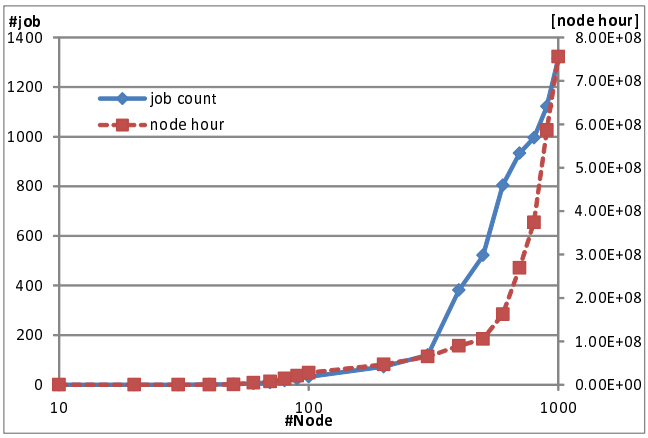


Figure 20.2: The number of jobs and system usage exceeding 25,000 [OPS]

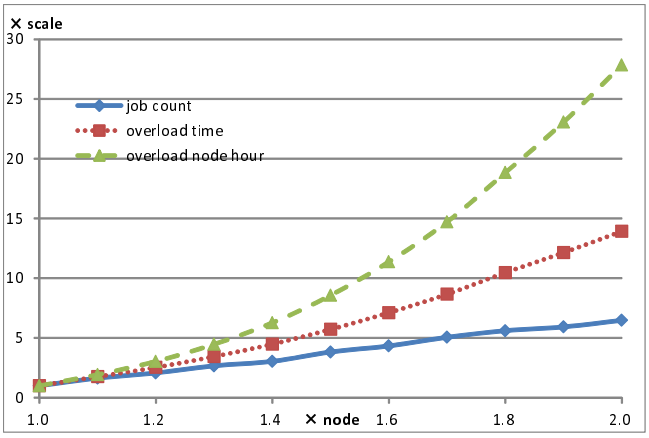


Figure 20.3: Changes in overload status for the number of job nodes

Previously, we tuned the single CPU performance using several techniques. Resultant performance was 0.461 PFLOPS using 82,944 nodes. Moreover, the K computer has been ranked 2nd on the ranking of HPCG. In this tuning, sustained memory throughput of 46 GB/s was obtained. Therefore, we must employ another tuning method to obtain higher performance.

In FY2016, we employed a method to decrease data transfer from memory. Due to this, 0.603 PFLOPS was obtained and the K computer was ranked 1st on the ranking of HPCG. In this method, two loops, a forward substitution loop and a backward substitution loop with the same coefficient matrix in the symmetric Gauss-Seidel (SYMGS) routine that is the most time-consuming routine are separated into total four loops. Those are the forward loop using only the upper triangle matrix, the forward loop using only the lower triangle matrix, the backward loop using only the lower triangle matrix, and the backward loop using only the upper triangle loop. Because the loop direction of the backward loop using the lower triangle matrix can be reversed without any arithmetic modification on the original formulation, two loops using the only lower triangle matrix can be fused. This fusion can reduce the data transfer of matrix values from memory.

This score is superior compared with other supercomputers on the list of TOP500 computing systems that have shown much better performance than the K computer.

This effort was reported at the HPCG BoF at The International Conference for High Performance Computing, Networking, Storage and Analysis 2016 (SC16) held in Salt Lake City, [10].

20.3.4.2 High Performance Geometric Multigrid-Finite Volume (HPGMG-FV) Benchmarking

HPGMG-FV is a benchmark program provides a metric of computer performance. According to the HPGMG official website, HPGMG-FV is a benchmark designed to proxy the finite-volume-based geometric multigrid linear solvers found in adaptive mesh refinement (AMR)-based applications. We conducted parameter surveys with a few hundred compute nodes of the K computer to obtain the best set of parameter values to maximize the DOF/s values of the benchmark test using all 82,944 compute nodes. The DOF/s value is the score of HPGMG-FV benchmarking. We estimated the DOF/s value of an all node test based on the results of weak-scaling experiments with up to 3,072 compute nodes.

20.3.4.3 Support for Improving the Computational Efficiency of Full-node Application Programs

We continued to assist the Hoshi Laboratory of Tottori University to improve their application "Extra Large-Scale Electronic Structure calculation (ELSES)" to apply for the ACM Gordon Bell Prize. This is an application for quantum chemistry based on an order-N algorithm. In FY2016, we performed bug-fix and sophisticated the job-script for large-scale run. As a result, the problems that occur for large-scale job were fixed. These efforts were reported at the 7th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems [4].

20.3.4.4 Graph-based Economic Simulation

To study the behavior of economic networks, a graph-based algorithm was proposed. The algorithm propagates financial stress in a network based on actual transactions among domestic companies. To perform massive parameter-sweep calculations, we needed to reduce the turnaround time in a graph traversal. In FY2016, we furthermore surveyed related algorithms (e.g., top-down/bottom-up/hybrid algorithm) to reduce computation time. Moreover, toward the post-K computer, we launched and joined the new project: "Exploratory Challenges on Post-K computer (Study on multilayered multiscale space-time simulations for social and economical phenomena)" that was supported by MEXT. In this project, we plan to use not only graph-based algorithm but also an agent-based algorithm [2]. To efficiently develop new applications with new algorithms, we installed the Python environment and its numerical modules in the K computer.

20.3.5 Evidenced-based Performance Tuning

Typical performance improvements for an application comprise two steps: finding a bottleneck using profilers and rewriting the source code. These steps are a form of engineering; however, the performance is strongly influenced by slightly rewriting the source code. Eventually, we often use an ad hoc solution instead of engineering with sufficient investigation. Therefore, even if we have tips and know-how regarding performance optimizations of an application, it is difficult to systematically marshal this knowledge and reuse it for other similar applications. In FY2016, based on our previous studies, we developed a code comprehension assistance tool that includes several features (e.g., Fortran parser, tree/source viewer, and loop highlighting to emphasize

hot spots based on supervised machine learning). This tool has been distributed as part of the AICS software. This study was conducted in collaboration with the HPC Usability Research Team in RIKEN AICS.

20.4 Schedule and Future Plan

The Software Development Team was reorganized into the Application Tuning Development Team.

20.5 Publications

20.5.1 Journal Articles

[1] Yoshito Kitazawa, Akiyoshi Kuroda, Naoyuki Shida, Tomoya Adachi, and Kazuo Minami, *Evaluation of MPI communication performance using throughput on the K computer (in Japanese)*, (submitted).

[2] Yuichi Hirokawa, Noriaki Nishikawa, Toshiyuki Asano, Masaaki Terai, and Teruo Matsuzawa, *A study of real-time and 100 billion agents simulation using the Boids model*, Artificial Life Robotics, Volume 21, Issue 4, pp.525-530, (2016).

20.5.2 Conference Papers

[3] Kiyoshi Kumahata, and Kazuo Minami, *Case Study on the Running Time Fluctuations of Applications*, Academic eXchange for Information Environment and Stragegy 2016 (AXIES2016), Kyoto, (2016).

[4] Takeo Hoshi, Hiroto Imachi, Kiyoshi Kumahata, Masaaki Terai, Kengo Miyamoto, Kazuo Minami, and Fumiyoshi Shoji, *Extremely scalable algorithm for* 10^8*-atom quantum material simulation on the full system of the K computer*, Proceedings of the 7th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems conjunction with the International Conference for High Performance Computing, Networking, Storage and Analysys 2016 (SC16), pp.33-40, Salt Lake City, Uhtah, (2016).

[5] Yoshito Kitazawa, Akiyoshi Kuroda, Naoyuki Shida, Tomoya Adachi, and Kazuo Minami, *Evaluation of MPI communication performance using throughput on the K computer (in Japanese)*, IPSJ High Performance Computing Symposium (IPSJ HPCS2017), Kobe, 2017, pp.17-25, (2017).

[6] Akiyoshi Kudoda, Shunsuke Inoue, Kentaro Koyama, Ryuichi Sekizawa, and Kazuo Minami, *Development of Job Analysis System for Power-saving and Operational Improvement on the K computer (in Japanese)*, IPSJ SIG Technical Reports (HPC), 2016-HPC-156(7), pp.1-6, (2016).

[7] Akiyoshi Kudoda, Shunsuke Inoue, Ryuichi Sekizawa, and Kazuo Minami, *Analysis of the Load of Local Meta Data Server Access from the Job I/O on the K computer (in Japanese)*, IPSJ SIG Technical Reports (HPC), 2017-HPC-160(27), pp.1-6, (2017).

[8] Masatomo Hashimoto, Masaaki Terai, Toshiyuki Maeda, and Kazuo Minami, *An Empirical Study of Computation-Intensive Loops for Identifying and Classifying Loop Kernels*, ICPE2017 Proceedings of the 8th ACM/SPEC on International Conference on Performance Engineering, pp.361-372, (2017).

[9] Hisashi Yashiro, Masaaki Terai, Ryuji Yoshida, Shin-ichi Iga, Kazuo Minami, and Hirofumi Tomita, *Performance Analysis and Optimization of Nonhydrostatic ICosahedral Atmospheric Model (NICAM) on the K computer and TSUBAME2.5*, Proceedings of the Platform for Advanced Scientific Computing Conference (PASC16), pp.3:1-3:8, (2016).

20.5.3 Posters and Presentations

[10] Kiyoshi Kumahata, Kazuo Minami, Akira Hosoi and Ikuo Miyoshi, *HPCG Performance Improvement on the K computer*, HPCG BoF at the International Conference for High Performance Computing, Networking, Storage and Analysis 2016 (SC16), Salt Lake City, Utah, (2016).

[11] Kiyoshi Kumahata, and Kazuo Minami, *A case study of the running time fluctuation of application*, The 4th International Workshop on Legacy HPC Application Migration (LHAM) conjunction with the 4th International Symposium on Computing and Networking (CANDAR), Higashi-Hiroshima, (2016).

[12] Kiyoshi Kumahata, *Introduction of runtime fluctuations*, The 95th AICS cafe, (2016).

[13] Kiyoshi Kumahata, *Some causes about performance fluctuations of applications*, The 6th Workshop on Joint Laboratory on Extreme Scale Computing (JLESC), Kobe, (2016).

[14] Akiyoshi Kudoda, Shunsuke Inoue, Kentaro Koyama, Ryuichi Sekizawa, and Kazuo Minami, *Improvement of the Usage of Computing Resources and Reduction of the Total Energy for Calculation on the K computer.*, 1st International Symposium on Research and Education of Computational Science (RECS), Tokyo, P4, (2016).

[15] Akiyoshi Kudoda, Shunsuke Inoue, Kentaro Koyama, Ryuichi Sekizawa, and Kazuo Minami, *Improvement of the Usage of Computing Resources and Reduction of the Total Energy for Calculation on the K computer (in Japanese)*, Academic eXchange for Information Environment and Strategy (AXIES2016), Kyoto, FA22, pp.1-8, (2016).

[16] Akiyoshi Kudoda, Shunsuke Inoue, Kentaro Koyama, Ryuichi Sekizawa, and Kazuo Minami, *Improvement of the Usage of Computing Resources and Reduction of the Total Energy for Calculation on the K computer*, The 7th AICS International Symposium, Kobe, P-28, pp.31, (2017).

[17] Tomomi Ohichi, Masaaki Terai, Mitsuo Yokokawa, and Kazuo Minami, *STView: An Eclipse Plug-in Tool for Visualizing Program Structures in Fortran Source Codes*, The International Conference for High Performance Computing, Networking, Storage and Analysis (SC16), Technical Program Posters, (2016).

20.5.4 Patents and Deliverables

[18] K-scope: Fortran source code analysis tool
http://www.aics.riken.jp/ungi/soft/kscope/

[19] CCB/EBT: Code comprehension assistance for evidence-based performance tuning
https://github.com/ebt-hpc/cca

[20] STView: An Eclipse plug-in Tool for Visualizing Program Structure in Fortran Source Codes
https://github.com/K-scope/STView

[21] 1PAtool: The tool on the K computer to display the results of the basic performance analysis and time breakdown analysis that are output as profile results by Precision PA visibility function
http://www.aics.riken.jp/en/k-computer/aics-software

Chapter 21

HPCI System Development Team

21.1 Members

Manabu Hirakawa (Team Leader)

Etsuya Shibayama (Visiting Scientist)

Osamu Tatebe (Visiting Scientist)

Manabu Higashida (Visiting Scientist)

Hiroshi Harada (Research & Development Scientist)

Akira Kondo (Technical Staff)

Chihiro Shibano (Technical Staff)

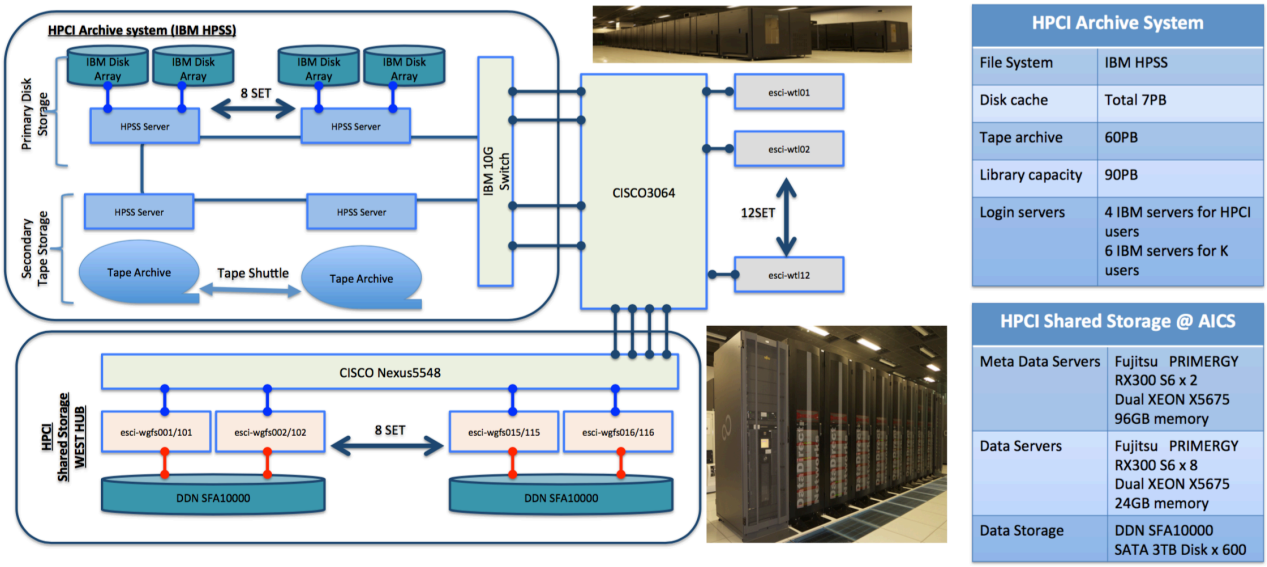
Hidetomo Kaneyama (Technical Staff)

Koichiro Ozaki (Technical Staff)

Satomi Yasuda (Assistant)

21.2 Research Activities

We are involved in the technical development of an innovative high performance computing infrastructure (HPCI) that will connect the major Japanese supercomputers installed in universities and research institutes, including the K computer, through a network. The computing environment realized by HPCI will meet the diverse needs of its intended users. Moreover, the high-speed network will enable the supercomputers, shared storage, and other functionalities of each HPCI system provider to operate as a common HPCI. Therefore, we are working on the technical side of the system operation, the technical coordination of the facilities comprising the HPCI system, and the operation of the HPCI shared storage (HPCI-SS) system. HPCI-SS is a large-scale distributed file system comprising four meta-data and 40 file-data servers. HPCI-SS forms the data-sharing infrastructure of HPCI led by the Ministry of Education, Culture, Sports, Science and Technology and provides a 22.5 PB single-view "Gfarm" network file system that is open to all HPCI users and supports scalable I/O performance in a geographically widely distributed environment. The HPCI-SS meta-data servers are located in RIKEN AICS and the University of Tokyo (U-Tokyo), whereas the file-data servers are located in AICS, U-Tokyo, and the Tokyo Institute of Technology (Tokyo Tech). HPCI-SS also supports single sign-on authentication, through which users can exchange their computational results present on their local storage systems with HPCI-SS without additional authentication. HPCI-SS has developed into a key infrastructure for the management and sharing of computational data in HPCI projects.



HPCI Archive System	
File System	IBM HPSS
Disk cache	Total 7PB
Tape archive	60PB
Library capacity	90PB
Login servers	4 IBM servers for HPCI users 6 IBM servers for K users

HPCI Shared Storage @ AICS	
Meta Data Servers	Fujitsu PRIMERGY RX300 S6 x 2 Dual XEON X5675 96GB memory
Data Servers	Fujitsu PRIMERGY RX300 S6 x 8 Dual XEON X5675 24GB memory
Data Storage	DDN SFA10000 SATA 3TB Disk x 600

Figure 21.1: Overview of HPCI Shared Storage and HPCI archive systems.

21.3 Research Results and Achievements

21.3.1 HPCI Shared Storage System

In FY2016, HPCI-SS was used by 78 HPCI projects and the total requested storage size was approximately two times the physical storage size. To cope with this demand, we allocated storage resources as follows:

- The maximum size of each project was set to 1.8 PB.
- The average number of file replicas was set to 1.5.

Figure 21.2 shows the HPCI-SS disk usage from FY2014 to FY2016. As seen in these graphs, although the HPCI-SS file usage was increasing, the disk usage was decreasing. This was a result of the new allocation policy. As shown in the figure 21.2, HPCI-SS was almost used up at the end of FY2016.

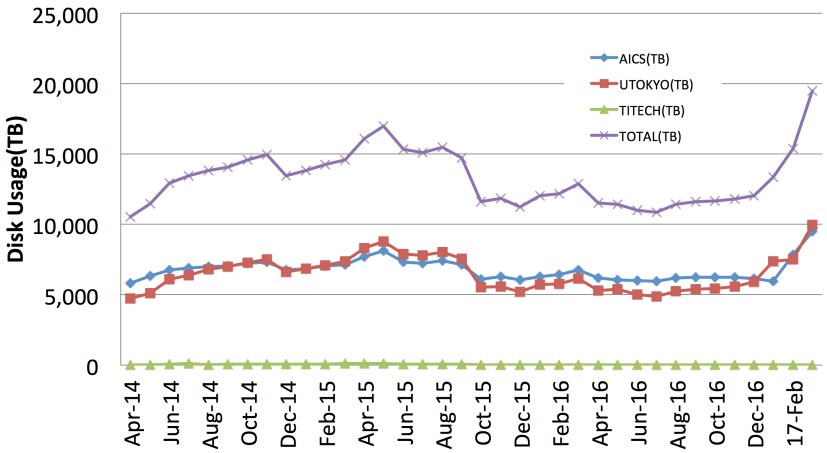


Figure 21.2: HPCI-SS disk usage.

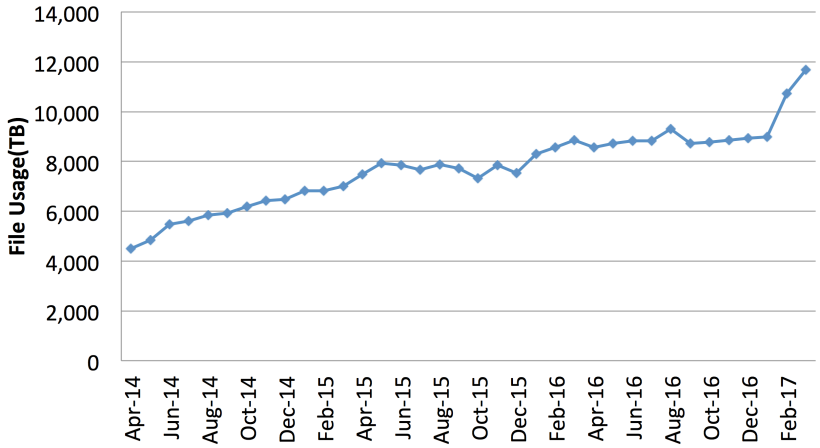


Figure 21.3: HPCI-SS file usage.

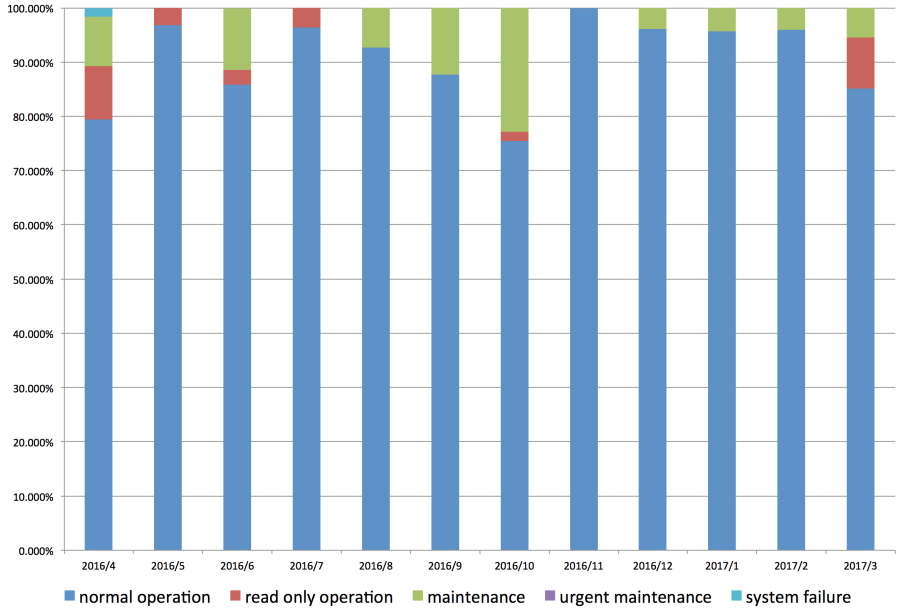


Figure 21.4: HPCI Shared Storage operation state.

21.3.2 Design of a Next-generation HPCI-SS System

The current system was introduced five years ago. To prepare for system deterioration, we plan to replace the existing system with a new one in FY2017. In FY2016, we designed the next-generation HPCI-SS system. First, to cope with an increase in the storage demand, we will provide a 50 PB storage to HPCI users.

To ensure the safety of data and allow for operation-time extension, all user data are recorded at RIKEN AICS and U-Tokyo. By duplexing data, we will able to continue uninterrupted system operation even if system failure occurs at U-Tokyo. We analyzed all system stop time and factor over the last four years of operation, and evaluated all system stops to determine whether service continuation was possible. Analysis results of system failure and maintenance time over the past four years indicate that 81% of the system stop time can be improved by duplexing data operation.

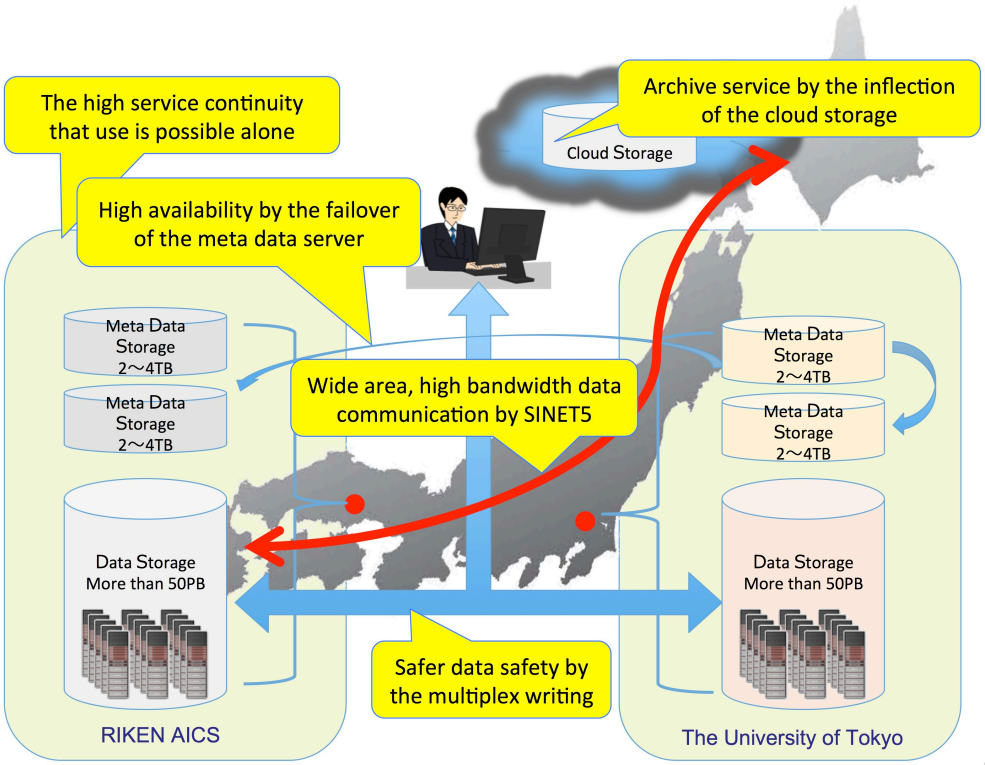


Figure 21.5: Next-generation HPCI Shared Storage System.

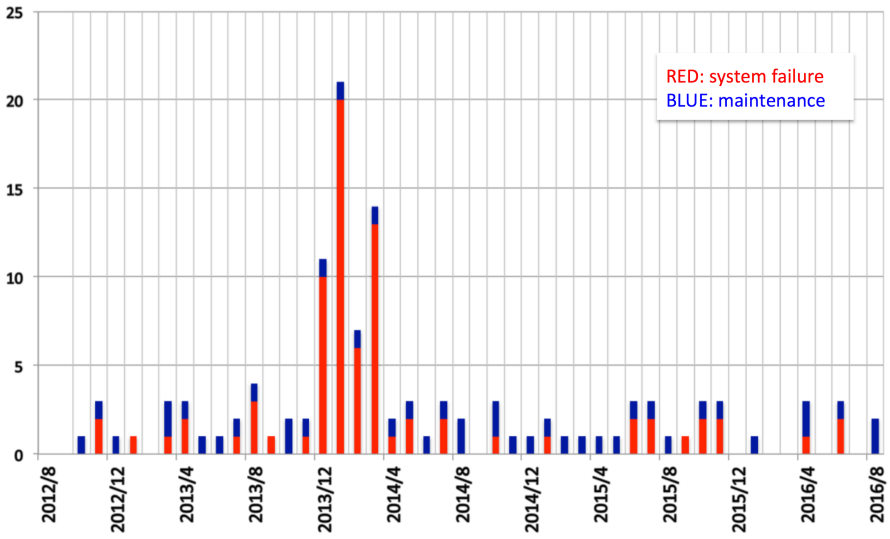


Figure 21.6: HPCI-SS service stop count.

21.3.3 Technological Planning and Coordination

For the technological planning and coordination processes listed below, we offer total technical support across the while operation the HPCI system and offer coordination for other HPCI system providers that are in the same operating environment.

- Oversee discussion tables for HPCI system providers.

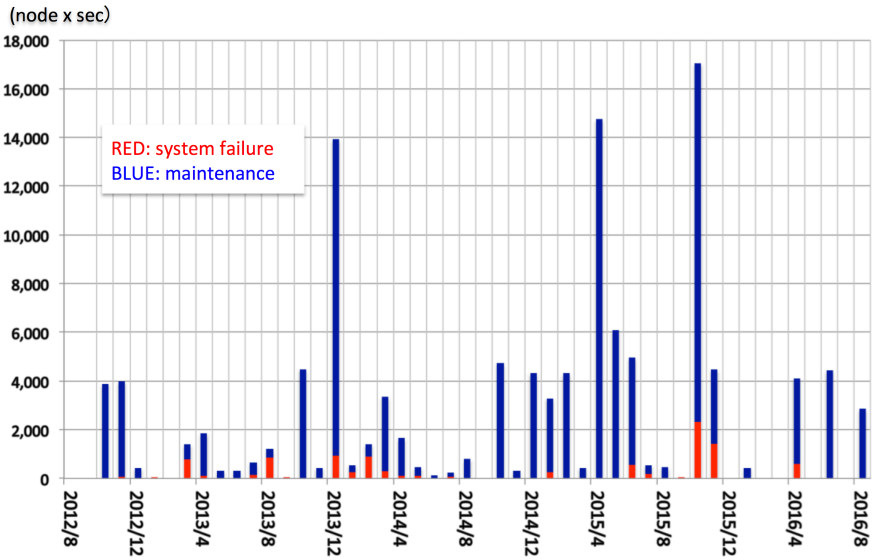


Figure 21.7: HPCI-SS service stop time.

- Conduct investigations and countermeasures for technical problems that arise while operating the HPCI system.
- Review software improvements that are related to the entire HPCI system.

We maintain the HPCI system operation such that it can accommodate various requests from users of those services. In addition we work with U-Tokyo, designated National University Corporation to maintain the HPCI-SS system. We provide data sharing and storage for the community and computational resources for the pre- and post-processing of data.
As shown in Figure 21.8, the computational resources in the HPCI system are provided by the supercomputer centers of nine universities, RIKEN AICS and the Japan Agency for Marine-Earth Science and Technology (JAMSTEC). The Joint Center for Advanced High Performance Computing (JCAHPC)has provided its resources since April 2017.

In FY2016, we coordinated and managed meetings for HPCI system providers and other relevant bodies.

- We hosted three meetings of the HPCI Cooperation Service Committee.
- We hosted eleven meetings of the HPCI Cooperation Service and Operation Working group.
- We hosted three meetings of the HPCI-SS Operation team.
- We hosted one meetings of the HPCI Security Incident Response Committee.

21.3.4 JIRA Ticket System

In FY2016, we intoroduced the JIRA ticket system to the HPCI Cooperation Service ansd Operation Working group. The main pourpose of introduction the JIRA system is to improve the quality of the HPCI system. The HPCI system been in operation since the past five years. Moreover, many universities and research organizations participate in HPCI. Therefore, it is difficult to maintain the HPCI system quality level without some types of tools.

Currently, the JIRA system has become indispensable for us, and is being widely used for system maintenance requests such as security patch application for certification server, approval matter management, and action item management. In FY2016, a total of 95 JIRA tickets were used by the HPCI Cooperation Service and Operation Working group.

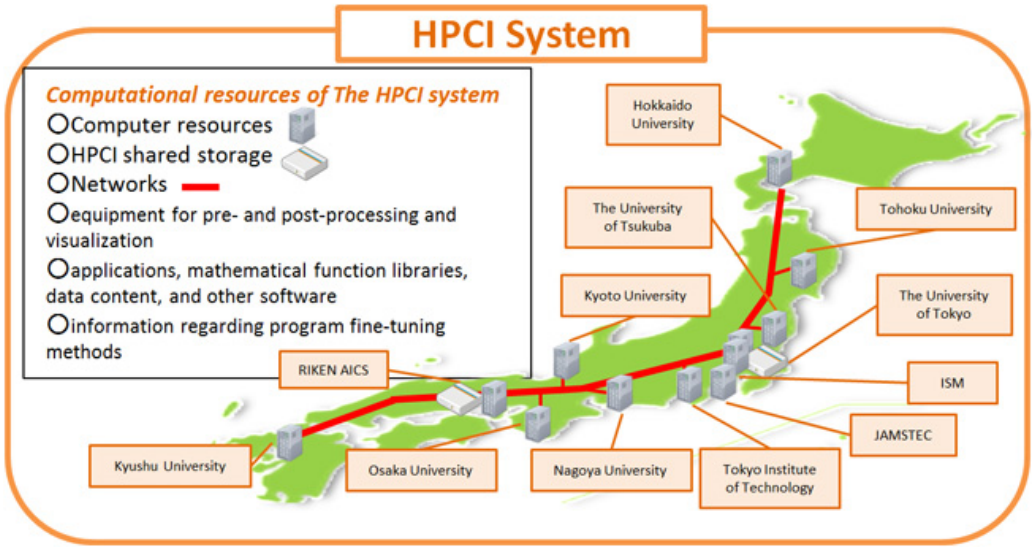


Figure 21.8: Overview of the HPCI structure.

Figure 21.9: HPCI JIRA screenshot.

21.3.5 HPCI System Monitoring

HPCI system monitoring allows us to monitor the status of the computing resources provided by each HPCI system provider, the operational status of the network, and the bandwidth and throughput performance of the system. HPCI system monitoring has the following duties:

- To investigate the causes of and response measures to technical problems that occur during the operation of the HPCI system.
- To research improvements in software related to the operation of the overall HPCI system.

- To operate and maintain the HPCI-SS site (the west site);
- To operate and manage the login gateway and the HPCI IdP of AICS (one of the HPCI system providers);
- To develop the HPCI online application system;
- To screen institutions seeking to participate in the shared operation (i.e., seeking to provide computing resources to the HPCI system) and check whether they satisfy the technical requirements.

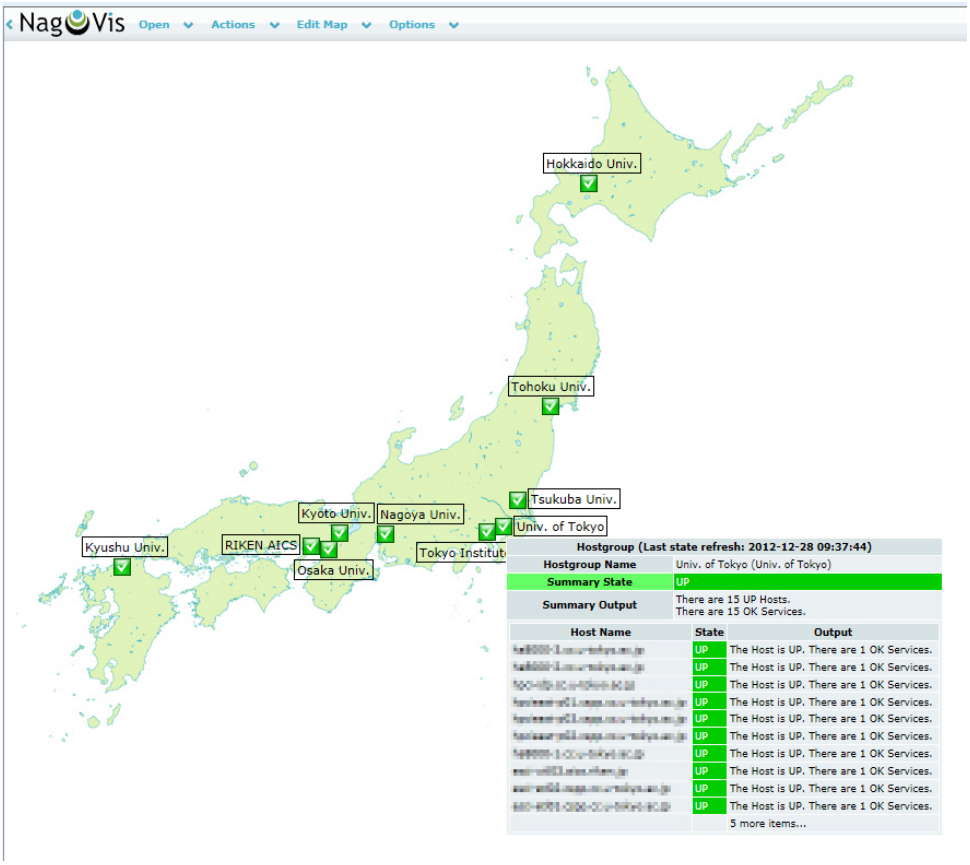


Figure 21.10: Overall Nagios/Nagvis monitoring system.

21.4 Schedule and Future Plan

21.4.1 Replacement of the Existing HPCI-SS System

From July to October 2017, the new 50 PB HPC-SS will be introduced, and the meta data servers will be reinforced. Almost 10 PB user data migration will be conducted from Octover 2017 to March 2018. We will provide the data migration method to the users to minimize the shutdown time.

21.4.2 Cloud Storage

Cold data so called as they are not accessed frequently, are stored in large quantities in HPCI-SS, and these cold data are the causes of the shortage of storage capacity. As these cold data do not necessarily have to be stored in a high-bandwidth storage system such as the new HPCI-SS, cloud storage is an effective measures for overcoming the capacity stringency. Therefore we will attempt to use cloud storage with HPCI-SS in FY2017. We will investigate cooperative work, data transfer bandwidth between cloud storage and HPCI-SS, and inflection example of the cloud storage in the research organization.

Part III

Flagship 2020 Project

Chapter 22

Flagship 2020 Project

22.1 Members

Primary members are only listed.

22.1.1 System Software Development Team

Yutaka Ishikawa (Team Leader)

Masamichi Takagi (Senior Scientist)

Atsushi Hori (Research Scientist)

Balazs Gerofi (Research Scientist)

Masayuki Hatanaka (Research & Development Scientist)

Takahiro Ogura (Research & Development Scientist)

Tatiana Martsinkevich (Postdoctoral Researcher)

Fumiyoshi Shoji (Research & Development Scientist)

Atsuya Uno (Research & Development Scientist)

Toshiyuki Tsukamoto (Research & Development Scientist)

22.1.2 Architecture Development

Mitsuhisa Sato (Team Leader)

Yuetsu Kodama (Senior Scientist)

Miwako Tsuji (Research Scientist)

Hidetoshi Iwashita (Research & Development Scientist)

Jinpil Lee (Postdoctoral Researcher)

Tetsuya Odajima (Postdoctoral Researcher)

Hitoshi Murai (Research Scientist)

Toshiyuki Imamura (Research Scientist)

Table 22.1: Development Teams

Team Name	Team Leader
Architecture Development	Mitsuhisa Sato
System Software Development	Yutaka Ishikawa
Co-Design	Junichiro Makino
Application Development	Hirofumi Tomita

22.1.3 Application Development

Hirofumi Tomita (Team Leader)

Yoshifumi Nakamura (Research Scientist)

Hisashi Yashiro (Research Scientist)

Seiya Nishizawa (Research Scientist)

Hiroshi Ueda Research (Scientist)

Yukio Kawashima (Research Scientist)

Naoki Yoshioka (Research Scientist)

Yiyu Tan (Research Scientist)

Soichiro Suzuki (Research & Development Scientist)

Kazunori Mikami (Research & Development Scientist)

22.1.4 Co-Design

Junichiro Makino (Team Leader)

Keigo Nitadori (Research Scientist)

Yutaka Maruyama (Research Scientist)

Takayuki Muranushi (Postdoctoral Researcher)

22.2 Project Overview

The Japanese government launched the FLAGPSHIP 2020 project [1] in FY 2014 whose missions are defined as follows:

- Building the Japanese national flagship supercomputer, the successor to the K computer, which is tentatively named the post K computer, and
- developing wide range of HPC applications that will run on the post K computer in order to solve the pressing societal and scientific issues facing our country.

RIKEN AICS is in charge of co-design of the post K computer and development of application codes in collaboration with the Priority Issue institutes selected by Japanese government, as well as research aimed at facilitating the efficient utilization of the post K computer by a broad community of users. Under the co-design concept, AICS and the selected institutions are expected to collaborate closely.

As shown in Table 22.1, four development teams are working on post K computer system development with the FLAGSHIP 2020 Planning and Coordination Office that supports development activities. The primary members are listed in Section 22.1.

The Architecture Development team designs the architecture of the post K computer in cooperation with Fujitsu and designs and develops a productive programming language, called XcalableMP (XMP), and its

[1] FLAGSHIP is an acronym for Future LAtency core-based General-purpose Supercomputer with HIgh Productivity.

tuning tools. The team also specifies requirements of standard languages such as Fortran and C/C++ and mathematical libraries provided by Fujitsu.

The System Software Development team designs and specifies a system software stack such as Linux, MPI and File I/O middleware for the post K computer in cooperation with Fujitsu and designs and develops multi-kernel for manycore architectures, Linux with light-weight kernel (McKernel), that provides a noise-less runtime environment, extendability and adaptability for future application demands. The team also designs and develops a low-level communication layer to provide scalable, efficient and portability for runtime libraries and applications.

The Co-Design team leads to optimize architectural features and application codes together in cooperation with AICS teams and Fujitsu. It also designs and develops an application framework, FDPS (Framework for Developing Particle Simulator), to help HPC users implement advanced algorithms.

The Application Development team is a representative of nine institutions aimed at solving Priority Issues. The team figures out weakness of target application codes in terms of performance and utilization of hardware resources and discusses them with AICS teams and Fujitsu to find out best solutions of architectural features and improvement of application codes.

22.3 Target of System Development and Achievements in FY2016

The post K's design targets are as follows:

- A one hundred times speed improvement over the K computer is achieved in maximum case of some target applications. This will be accomplished through co-design of system development and target applications for the nine Priority Issues.
- The maximum electric power consumption should be between 30 and 40 MW.

In FY2016, the second phase of the detailed design was completed. The major components of system software are summarized as follows:

- Highly productive programming language, XcalableMP
  XcalableMP (XMP) is a directive-based PGAS language for large scale distributed memory systems that combines HPF-like concept and OpenMP-like description with directives. Two memory models are supported: global view and local view. The global view is supported by the PGAS feature, i.e., large array is distributed to partial ones in nodes. The local view is provided by MPI-like + Coarray notation.
- Domain specific library/language, FDPS
  FDPS is a framework for the development of massively parallel particle simulations. Users only need to program particle interactions and do not need to parallelize the code using the MPI library. The FDPS adopts highly optimized communication algorithms and its scalability has been confirmed using the K computer.
- MPI + OpenMP programming environment
  The current de facto standard programming environment, i.e., MPI + OpenMP environment, is supported. Two MPI implementations are being developed. Fujitsu continues to support own MPI implementation based on the OpenMPI. RIKEN is collaborating with ANL (Argonne National Laboratory) to develop MPICH, mainly developed at ANL, for post K computer. In FY2016, we fixed the issue that launching many processes took unacceptable time on a large scale manycore-based cluster such as OakForest-PACS. Other achievements[3] have been described in Section 1.3.1.
- New file I/O middleware
  The post K computer does not employ the file staging technology for the layered storage system. The users do not need to specify which files must be staging-in and staging-out in their job scripts in the post K computer environment. The LLIO midleware, employing asynchronous I/O and caching technologies, has been being designed by Fujitsu in order to provide transparent file access with better performance. The functional design of LLIO was completed in FY2016.
- Application-oriented file I/O middleware
  In scientific Big-Data applications, such as real-time weather prediction using observed meteorological data, a rapid data transfer mechanism between two jobs, ensemble simulations and data assimilation,

is required to meet their deadlines. In FY2016, a framework called Data Transfer Framework (DTF), based on PnetCDF file I/O library, that silently replaces file I/O with sending the data directly from one component to another over network was designed and its prototype system was implemented and evaluated. The detailed achievement[4] has been described in Section 1.3.2.

- Process-in-Process
  "Process-in-Process" or "PiP" in short is a user-level runtime system for sharing an address space among processes. Unlike the Linux process model, a group of processes shares the address space and thus the process context switch among those processes does not involve hardware TLB flushing. It was implemented in FY2016, and its applicability to a communication mechanism has been tested. The detailed achievement has been described in Section 1.3.4.

- Multi-Kernel for manycore architectures
  Multi-Kernel, Linux with light-weight Kernel (McKernel) is being designed and implemented. It provides: i) a noiseless execution environment for bulk-synchronous applications, ii) ability to easily adapt to new/future system architectures, e.g., manycore CPUs, a new process/thread management, a memory management, heterogeneous core architectures, deep memory hierarchy, etc., and iii) ability to adapt to new/future application demands, such as Big-Data and in-situ applications that require optimization of data movement. In FY2016, McKernel was improved for NUMA CPU architectures. The detailed improvements have been described in Section 1.3.5.

It should be noted that these components are not only for post K computer, but also for other manycore-based supercomputer, such as Intel Xeon Phi.

22.4 International Collaborations

22.4.1 DOE/MEXT Collaboration

The following research topics were performed under the DOE/MEXT collaboration MOU.

- Optimized Memory Management
  This research collaboration explores OS supports for deep memory hierarchies. In FY2016, the movepages system call was parallelized in McKernel and its applicability for a manycore processor with two memory hierarchies, KNL, was evaluated using a simple stencil code.

- Efficient MPI for exascale
  In this research collaboration, the next version of MPICH MPI implementation, mainly developed by Argonne National Laboratory (ANL), has been cooperatively developed. The FY2016 achievements have been described in the previous section.

- Dynamic Execution Runtime
  This research collaboration shares designs for asynchronous and dynamic runtime systems. In FY2016,

- Metadata and active storage
  This research collaboration, run by the University of Tsukuba as contract, studies metadata management and active storage.

- Storage as a Service
  This research collaboration explores APIs for delivering specific storage service models. This is also run by the University of Tsukuba.

- Parallel I/O Libraries
  This research collaboration is to improve parallel netCDF I/O software for extreme-scale computing facilities at both DOE and MEXT. To do that, the RIKEN side has designed DTF as described in the previous section.

- OpenMP/XMP Runtime
  This research collaboration explores interaction of Argobots/MPI with XscalableMP and PGAS models.

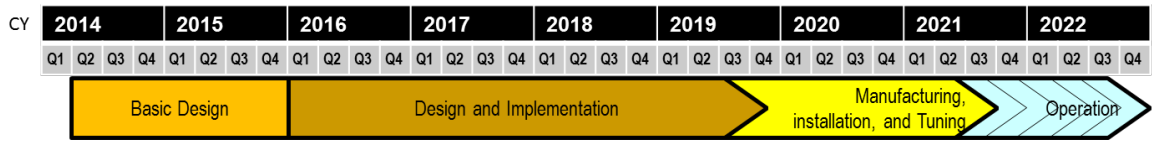


Figure 22.1: Schedule

- Exascale co-design and performance modeling tools
  This collaborates on an application performance modeling tools for extreme-scale applications, and shared catalog of US/JP mini-apps.
- LLVM for vectorization
  This research collaboration explores compiler techniques for vectorization on LLVM.
- Power Monitoring and Control, and Power Steering
  This research collaboration explores APIs for monitoring, analyzing, and managing power from the node to the global machine, and power steering techniques for over-provisioned systems are evaluated.

22.4.2 CEA

RIKEN and CEA, Commissariat *à* l'*é*nergie atomique et aux *é*nergies alternatives, signed MOU in the fields of computational science and computer science concerning high performance computing and computational science in January 2017. The following collaboration topics are now taken into account:

- Programming Language Environment
- Runtime Environment
- Energy-aware batch job scheduler
- Large DFT calculations and QM/MM
- Application of High Performance Computing to Earthquake Related Issues of Nuclear Power Plant Facilities
- Key Performance Indicators (KPIs)
- Human Resource and Training

22.5 Schedule and Future Plan

As shown in Figure 22.1, the design and prototype implementations will be done before the end of 2019, and the system will be deployed after this phase. The service is expected to start public operation at the range from 2021 to 2022.

22.6 Publications

22.6.1 Conference Papers

[1] Y. Kawashima, K. Sawada, T. Nakajima, and M. Tachikawa. Journal of Computer Chemistry, (15):203209, 2016.
[2] Y. Nakamura, Y. Kuramashi, S. Takeda, and A. Ukawa. Critical endline of the Finite temperature phase transition for 2+1 avor QCD around the SU(3)-avor symmetric point. PHYSICAL REVIEW D, (94, 114507).

[3] Masayuki Hatanaka, Takahiro Ogura, Masamichi Takagi, Atsushi Hori, and Yutaka Ishikawa. Prototype implementation and evaluation of an mpi persistent neighborhood collective operation using tofu2 protocol offlaoding capability. In IPSJ SIG Technical Report, volume 2016-HPC-157, December 2016. (In Japanese).
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