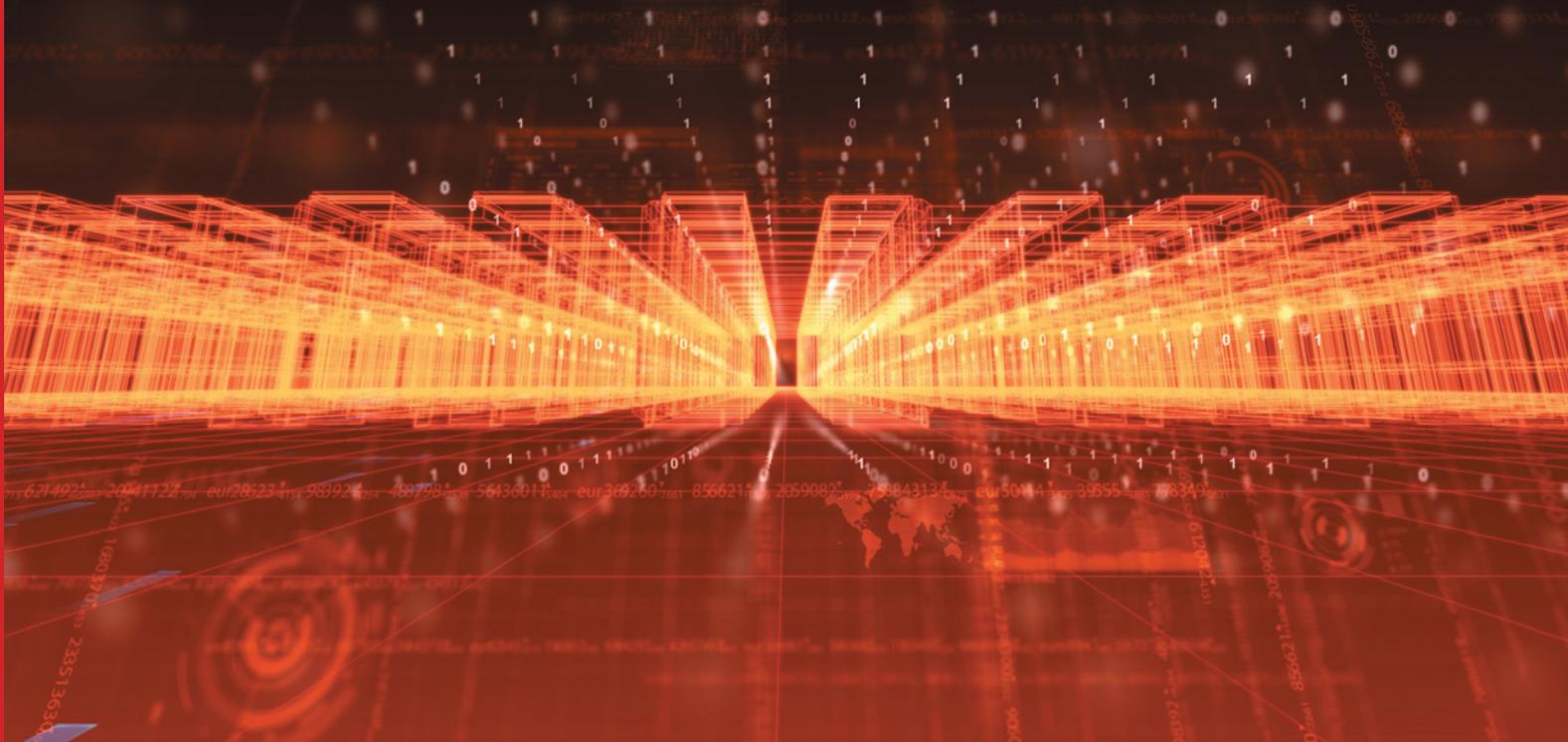


RIKEN AICS

Research Division



Computer simulations
create the future



RIKEN
Advanced Institute for
Computational Science

Overview

Division Director's Message

The AICS Research Division, which is composed of a number of research teams in computational and computer sciences, aims to be a global center achieving significant advances in science and technology through interdisciplinary collaboration across the two disciplines.

Supercomputers execute an enormous volume of computations using millions of cores simultaneously and in parallel. Developing supercomputers and extracting their full capability require close collaboration between Computational Science, which uses supercomputers, and Computer Science, which develops them. In addition to carrying out frontier research, the research teams pursue cross-disciplinary studies and develop software for advanced usage of the supercomputer K.

With the launch of the post K computer project in 2014, the Research Division is actively collaborating with the project team to carry out the co-design of the post-K computer.

Through these activities, the Research Division is making new strides in the development of supercomputers, which have become truly indispensable in broad areas of science and technology ranging from particles and the universe, materials, the global environment, life and medicine, to engineering, along with frontier research in science and technology making full advantage of these powerful machines.



Akira Ukawa

Deputy Director
RIKEN Advanced Institute for Computational Science
Division Director
RIKEN AICS Research Division

Basic Concepts of AICS

AICS aims to establish the science of forecasting based on computer simulation. To this end, AICS does the following:

Manage the operations of the K computer and maintain a user-friendly environment.

Generate cutting-edge scientific results and technological breakthroughs by promoting collaborations and the integration of computational and computer science as an international center of excellence.

Develop the post-K supercomputer and application software for it based on a roadmap for the future of computational science.





Director
Kimihiko Hirao



Deputy Director
Akira Ukawa



Deputy Director
Shigeo Okaya

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Collaboration with Domestic and International Institutions

RIKEN promotes collaboration with universities, research institutions and private corporations in Japan and overseas for ensuring that research achievements are disseminated widely throughout society. RIKEN AICS has agreements with many institutions and organizations for joint research and collaboration.

- Joint research:
45 universities, research institutions, private enterprises, etc. (of which three are overseas entities)
- Research agreements:
13 (of which 10 are with overseas entities)

As of September 2017

Major collaborating institutions and organizations

Japan	Kobe University, University of Tsukuba, Tohoku University
USA	National Center for Supercomputing Applications (NCSA), University of Illinois University of Maryland (UMD)
UK	University of Reading (UoR)
Italy	Scuola Internazionale Superiore di Studi Avanzati (SISSA)
France	Centre national de la recherche scientifique (National Center for Scientific Research) (CNRS) Commissariat à l'énergie atomique et aux énergies alternatives (Alternative Energies and Atomic Energy Commission) (CEA)
Germany	Jülich Supercomputing Center, Jülich Research Institute (JSC)
Australia	National Computational Infrastructure (NCI), Australia National University
China	Beijing Computational Science Research Center (CSRC)
Other	Joint Laboratory for Extreme-Scale Computing (JLESC) (made up of six research institutes in France, Spain, Germany and the United States)

Note: For more information on collaboration with RIKEN AICS, please contact the Collaborations Group, Computational Science Planning Office. (P23)



System Software Research Team

Team Leader **Yutaka Ishikawa** yutaka.ishikawa@riken.jp

Team Website <http://www-sys-aics.riken.jp>

Development of Novel System Software for HPC, Big Data and AI

Our research team is responsible for developing an advanced system software stack's. We are also conducting research and development for the K computer, its successor the post-K computer, and for future systems, taking into consideration continuity of the user environment and usability. The software stack under development is made up of the following:

• OS kernel

We are developing a lightweight kernel, called Mckernel, for multi-core type parallel computers. Applications running on Linux run on Mckernel without recompilation. Mckernel is running on Intel's latest Xeon Phi processor: Knights Landing (KNL).

• MPI communication library

We have implemented the MPICH communication library, an implementation of the MPI communication library developed mainly by Argonne National Laboratories, on the K and post-K computers. In particular, we are developing a mechanism that can efficiently use post-K computer communication hardware.

• File I / O library

We are developing a DTF file I/O library, realizing a real-time job-to-job file I/O and a FTAR file I/O library, and parallelizing a file I/O with the tar format.

Career of Team Leader

- 2014 Team Leader, System Software Research Team and System Software Development Team, Leader of Flagship 2020 Project, AICS, RIKEN (-present)
- 2006 Professor, The University of Tokyo
- 1987 ElectroTechnical Laboratory (currently reorganized as AIST)
- 1987 Doctor, Electrical Engineering from Keio University

Publications

1. M. Hatanaka, M Tanaka, A.Hori and Y.Ishikawa.: "Offloaded MPI Persistent Collectives using Persistent Generalized Request Interface," EuroMPI/ USA 2017, (2017).
2. B.Gerofi, M.Takagi, G.Nakamura, T.Shirasawa, A. Hori and Y. Ishikawa.: "On the Scalability, Performance Isolation and Device Driver Transparency of the IHK/Mckernel Hybrid Lightweight Kernel," IEEE International Parallel and Distributed Processing Symposium (IPDPS), (2016).
3. M. Si, A. J. Pena, Hammond, P. Balaji, M. Takagi and Y. Ishikawa.: "Casper: An Asynchronous Progress Model for MPI RMA on Many-Core Architectures," Proceedings of 2015 IEEE International Parallel and Distributed Processing Symposium (IPDPS), pages 665-676, 2015.

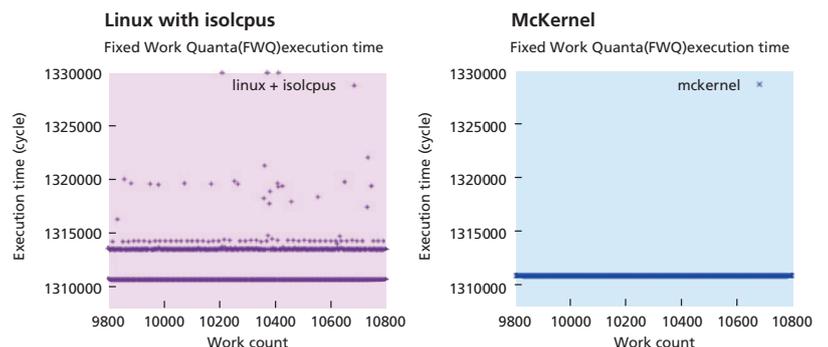
Recent Achievement

Development of Mckernel: a Linux-compatible lightweight kernel

Extreme degrees of parallelism and deep memory hierarchies in high-end computing require a novel runtime environment so that large-scale bulk-synchronous parallel applications run efficiently. An advanced runtime environment has been historically achieved by deploying lightweight kernels, though they are only able to provide a restricted set of the POSIX API. However, the increasing prevalence of more complex application constructs, such as in-situ analysis and workflow composition, dictates the need for the rich APIs of POSIX and Linux. In order to comply with these seemingly contradictory requirements, we are designing and implementing hybrid kernels, where Linux and a lightweight kernel are run side-by-side on compute nodes. We are developing a lightweight kernel called Mckernel, and the interface between it and the Linux kernel is called IHK.

Mckernel is booted from the Linux kernel without hardware rebooting. It retains a binary compatible interface with Linux, i.e., the same Linux binary runs on Mckernel; however, it implements only a small set of per-

formance-sensitive system calls, such as memory/process/thread management, the rest being delegated to Linux. One of the significant results, noise-less environment, is shown in the Figure below. The Fixed Work Quanta benchmark, provided by Sandia National Laboratory, reports how much execution times of fixed workloads deviate. The result shows that the fixed execution time in Mckernel is almost constant, whereas a large deviation is observed in Linux.



Results of Fixed Work Quanta (FWQ)



Programming Environment Research Team

Team Leader **Mitsuhsa Sato** msato@riken.jp

Team Website <http://pro-env.riken.jp>

Improving the Performance and Productive Programming Environment for Exascale and Beyond

We are researching and developing parallel programming models and a new programming language to exploit the full potential of large-scale parallelism on the K computer, as well as working to increase productivity of parallel programming. The new programming language, called XcalableMP (XMP), is based on the PGAS (Partitioned Global Address Space) model, which was originally designed by the Japanese HPC language research community. We are working on a reference XMP compiler, the Omni XMP compiler, and have deployed it on the K computer for users, where it has several optimizations. We are also conducting a performance study of the PGAS language, as well as developing an extension for an accelerator cluster for use beyond the K computer. As for performance tuning tools for large-scale scientific applications running on the K computer, we have ported the Scalasca performance-tuning and analysis tool and we are examining its potential.

Regarding improving the performance, and productive programming model, we are working on a new version of XcalableMP: XcalableMP 2.0; it will include support for large-scale many-core clusters by multitasking with the PGAS model. This programming model will reduce synchronization overhead, thereby eliminating time-consuming global synchronization; enable the overlap of computation and communication in many-core processing; and reduce communications overhead of the RDMA feature. We are also developing the Omni compiler as part of the infrastructure for source-to-source transformation for high-level optimization, and we are optimizing many core processing and wide SIMD for the post-K supercomputer.

Career of Team Leader

- 2014 Team Leader, Architecture Development Team of Flagship 2020 Project, AICS, RIKEN (-present)
- 2010 Team Leader, Programming Environment Research Team, AICS, RIKEN (-present)
- 2007 Director, Center for Computational Sciences, University of Tsukuba
- 2001 Professor, Graduate School of Systems and Information Engineering, University of Tsukuba (-present)
- 1996 Chief of Parallel and Distributed System Performance Laboratory in Real World Computing Partnership, Japan.

Publications

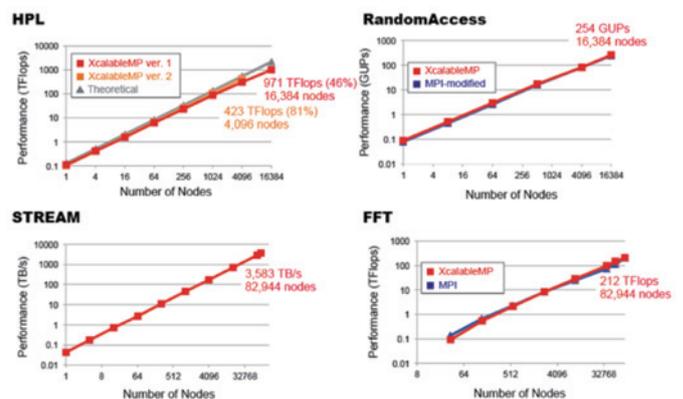
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- M. Tsuji, M. Sato. "Fault Tolerance Features of a New Multi-SPMD Programming/Execution Environment," Proceedings of First International Workshop on Extreme Scale Programming Models and Middleware, Texas, USA, Nov. 2015. doi: 10.1145/2832241.2832243

Recent Achievement

XcalableMP received HPC best performance awards at SC13 and SC14 In recent years our XcalableMP received the HPC Challenge Class 2 Award at SC13, and the HPC Challenge Class 2 Best Performance Award at SC14. The HPC Challenge Class 2 is a competition to determine the programming language that achieves the highest productivity and performance. The HPC benchmarks are a set of benchmarks to evaluate multiple attributes of an HPC system: RandomAccess, Fast Fourier Transform (FFT), High Performance Linpack (HPL), and STREAM. All four have been implemented on the K computer using XcalableMP. In addition, the Himeno Benchmark, which is a typical stencil application, has also been implemented.

We submitted the results to the SC13 and SC14 HPC Challenge Benchmark Class2 Competition. In order to evaluate their performance, we used all K computer nodes to the maximum. We then fine-tuned the Omni Compiler for the K computer and for the HPC benchmarks after SC13. The Figure below shows the performance results at SC14. We demonstrated that the performances of XcalableMP implementations are almost the same as those of the reference implementations by MPI. As a metric to measure productivity, the source lines of code of our implementations are smaller than

those of the reference implementations using MPI. Through these implementations and performance evaluations, we demonstrated that XcalableMP improves productivity and performance.



XcalableMP performance results measured against HPC benchmarks (SC14)



Processor Research Team

Team Leader **Kentaro Sano** kentaro.sano@riken.jp

Team Website <http://www.riken.jp/en/research/labs/aics/research/processor/>

Developing Parallel-computing Models and Acceleration Technologies for Large-scale High-performance Computing

To achieve high-performance computing with the K computer, we need to use more than 80,000 networked computing nodes in a way that they cooperate with each other using communication data. However, the overall performance may be degraded by the considerable overhead required for global communications and synchronization among the nodes. We are developing computing accelerators to achieve large-scale processing with less performance degradation by introducing a new parallel computing model based on a "Data-Flow" model with localized communication and synchronization. Also, we are developing data-flow accelerators where custom-computing circuits are automatically generated by a high-level synthesis compiler for each target application. Such specially customized hardware structures allow us to achieve high performance processing even for those applications which conventional CPUs are not good at handling. These research results are helping advance usage of the K computer, as well as aiding exploration of new computing models and new architectures for future supercomputers.

Career of Team Leader

- 2017 Team Leader, Processor Research Team, AICS, RIKEN (-present)
- 2006 Visiting Researcher, Imperial College, London
- 2005 Associate Professor, Graduate School of Information Sciences, Tohoku University
- 2000 Graduated from Computer and Mathematical Sciences, Graduate School of Information Sciences, Tohoku University

Publications

1. K. Sano and S. Yamamoto, "FPGA-based Scalable and Power-Efficient Fluid Simulation using Floating-Point DSP Blocks," IEEE Transactions on Parallel and Distributed Systems (TPDS), DOI: 10.1109/TPDS.2017.2691770, (2017).
2. T. Ueno, K. Sano, and S. Yamamoto, "Memory Bandwidth Compressor for FPGA-based High-Performance Custom Stream Computation," ACM Transactions on Reconfigurable Technology and Systems (TRET), (2017).
3. K. Nagasu, K. Sano, F. Kono, and N. Nakasato, "FPGA-based Tsunami Simulation: Performance Comparison with GPUs, and Roofline Model for Scalability Analysis," Journal of Parallel and Distributed Computing, DOI:10.1016/j.jpdc.2016.12.015, (2016).

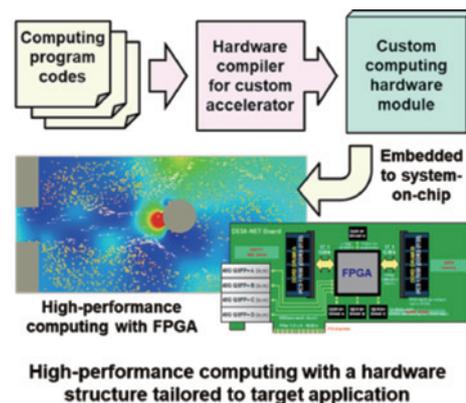
Research Content

Low-power and high-performance numerical computing using our own hardware compiler to generate custom-computing acceleration As the advancement of semiconductor technology based on Moore's Law slows down, it will be difficult to improve computing performance with multi-core microprocessors in the near future. One of the promising solutions to solve this problem is a reconfigurable custom computing machine, where software code of a target application is converted to run on customized accelerator hardware implemented and executed with field-programmable gate arrays (FPGAs).

To date, we have developed a high-level synthesis compiler to generate stream-computing hardware modules with a data-flow computing model, as well as a system to execute high-performance computing with the generated modules implemented on FPGAs. In the case of a tsunami simulation, for instance, we achieved two times higher sustained performance and an eight-fold improvement in power performance using FPGAs compared with GPUs. These improvements were achieved by employing efficient subsystem structures tailored to the target application, including customized memory subsystems and data-paths with increased pipelines.

In addition, we have developed a real-time data-compression hardware module using multiple FPGAs to enhance memory and network bandwidth for high performance computing.

Going forward, we will further advance these developments, and also develop a new system to easily achieve high performance with massively-large-scale and complex computers. We aim to establish a new computing model and architecture for high-performance computing in the Post-Moore era.





Large-scale Parallel Numerical Computing Technology Research Team

Team Leader **Toshiyuki Imamura** imamura.toshiyuki@riken.jp

Team Website <http://www.aics.riken.jp/labs/lpnctr/index.html>

Developing a Numerical Library for Fast, High-precision Simulation

To utilize the full computing potential of the K computer and post-K computer, and to produce simulations with higher efficiency and accuracy, it is necessary to take advantage of numerical software libraries that have been tuned to the needs of computer science and applied mathematics. We are researching and developing a large-scale, high-performance numerical library called KMATHLIB. Typical library algorithms commonly employed in simulation programs are used to handle systems of linear equations, eigenvalue calculations, three-dimensional Fast Fourier transforms, and long-period random number generators. We maintain corresponding library algorithms such as EigenExa, KMATH_FF-T3D, and KMATH_RANDOM. We are modifying the existing KMATHLIB algorithms for use as a component of KMATHLIB2, which works in a scalable manner on the post-K computer.

Furthermore, we are promoting R&D of innovative algorithms that can deal with the unprecedented challenges raised by the K computer, such as the eigenvalue problem of a nonsymmetric matrix, and higher order tensor calculations. In addition to the modification and development of such algorithms, we are extending a high-precision calculation framework developed for the K computer to use on the post-K computer. We have also developed a method to reduce accumulated errors, and which guarantees the reproducibility of calculations by controlling the number of effective digits and removing non-determinism hidden in parallel calculations and when repeating these calculations. Collaboration is another important issue. We are collaborating with researchers and companies in Japan and overseas with the aim of establishing fundamental technologies for numerical libraries that can continue to be used well into the future.

Career of Team Leader

- 2012 Team leader, Large-scale Parallel Numerical Computing Technology Research Team, AICS, RIKEN (-present)
- 2003 Assistant Professor, University of Electro-Communications
- 1996 Researcher, Japan Atomic Energy Research Institute
- 1996 Graduated from Applied Systems and Science, Graduate School, Division of Engineering, Kyoto University

Publications

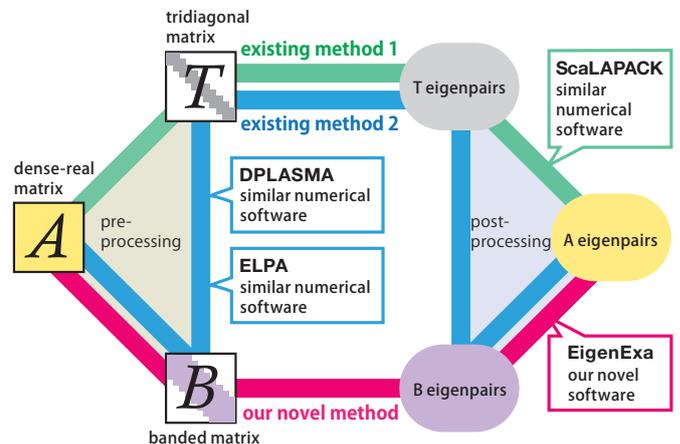
1. T. Imamura, T. Fukaya, Y. Hirota, S. Yamada and M. Machida, "CAHTR: Communication-Avoiding Householder TRidiagonalization", Proc. ParCo2015, Advances in Parallel Computing, Vol. 27: Parallel Computing: On the Road to Exascale, pp. 381-390, 2016.
2. Y. Hirota and T. Imamura, "Divide-and-Conquer Method for Banded Generalized Eigenvalue Problems", Journal of Information Processing Computing System, Vol.52, Nov, 20, 2015.
3. T. Fukaya and T. Imamura.: "Performance evaluation of the EigenExa eigensolver on Oakleaf-FX: tridiagonalization versus pentadiagonalization" Parallel and Distributed Processing Symposium Workshop (IPDPSW), 2015 IEEE International, pp. 960-969, May 25 2015.

Recent Achievement

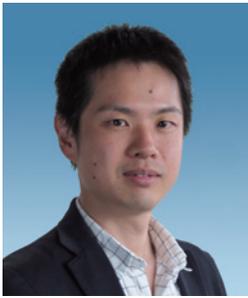
World Largest Dense Eigenvalue Computation The solution of real symmetric dense Eigen value problems is one of the fundamental matrix computations. To date, several new high-performance Eigen solvers have been developed for peta and postpeta scale systems. One of these, the Eigen Exa Eigen solver, has been developed in Japan. Eigen Exa provides two routines: eigens, which is based on traditional tridiagonalization, and eigensx, which employs a new method via a pentadiagonal matrix. Recently, we conducted a detailed performance evaluation of Eigen Exa by using 4,800 nodes of the Oak leaf-FX supercomputer system. In this paper, we report the results of our evaluation, which is mainly focused on investigating the differences between the two routines.

The results clearly indicate both the advantages and disadvantages of eigensx over eigens, which will contribute to further performance improvement of Eigen Exa. The obtained results are also expected to be useful for other parallel dense matrix computations, in addition to Eigen value problems. We have successfully solved a world largest-scale dense eigenvalue problem (one million dimension) by EigenExa taking advantage of the overall nodes (82,944 processors) of K computer in 3,464 seconds. Our EigenExa achieves

1.7 PFLOPS (16% of the K computer's peak performance). It is the world highest performance for solving an eigenvalue problem of a dense matrix.



Schematic view of a new scheme



HPC Usability Research Team

Team Leader **Hiroya Matsuba** hiroya.matsuba@riken.jp

We Aim to Make Programming of Simulations and Data Analysis and Their Combinations More Efficient

Our mission is to improve programming productivity for supercomputers. Raising super-computer-programming efficiency is important because of the growing need to rapidly simulate various real-world events and phenomena. Going forward, rapid simulation will become even more necessary, as it is expected to be an essential tool for artificial intelligence, given simulations provide virtual environments in which AI can learn. Additionally, simulation aids more practical data analysis because it can generate data of rare events.

We are researching programming techniques to combine existing tools and frameworks for simulation, data analysis, and machine learning, as well as preparing such tools for use on the K computer. We are also developing a new computer language that employs highly abstract descriptions to make use of these tools and frameworks. This will enable users to conduct simulations, data analysis, and their combinations with less development effort than is required today.

We are also collaborating with industry. Considering the fact that the industrial trend is shifting from making products to providing services, we believe academic institutions should provide our research results to users as a service. In order to promote this goal, we are investigating not only the most efficient programming techniques, but also what will produce the most practical benefits for users.

Career of Team Leader

- 2017 Team Leader, HPC Usability Research Team, AICS, RIKEN (-present)
- 2012 Visiting Researcher, AT&T Labs Inc. (-2014)
- 2010 Researcher, Hitachi, Ltd.
- 2010 Ph.D. in Computer Science, The University of Tokyo
- 2006 Research Associate, The University of Tokyo

Publications

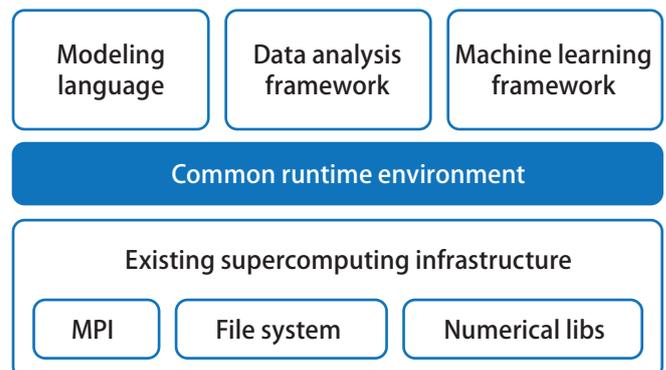
1. Hiroya Matsuba, Kaustubh Joshi, Matti Hiltunen and Richard Schlichting, "Airfoil: A Topology Aware Distributed Load Balancing Service," 2015 IEEE 8th International Conference on Cloud Computing
2. Hiroya Matsuba, Matti Hiltunen, Kaustubh Joshi and Richard Schlichting, "Discovering the Structure of Cloud Applications Using Sampled Packet Traces," 2014 IEEE International Conference on Cloud Engineering
3. Atsushi Hori, Yoshikazu Kamoshida, Hiroya Matsuba, Kazuki Ohta, Takashi Yasui, Shinji Sumimoto and Yutaka Ishikawa, "On-demand file staging system for Linux clusters," 2009 IEEE International Conference on Cluster Computing

Research Content

Modeling languages for supercomputers We are researching how to make use of modeling languages in supercomputers. We believe the most important issues in supercomputing are the complexities and difficulties involved in developing simulations, especially in the area of describing models of target objects and phenomena. While modeling languages are of some practical use in dealing with these issues, programs written with such languages are usually slower than lower-level computer languages. To increase both productivity and efficient execution, we are, for example, connecting a highly productive modeling language to a numerical library for supercomputers.

Combining Simulation with Data Analysis As well as realizing efficient execution of simulations written in a modeling language, we are extending the modeling language so that it can describe how to use data processing programs. By using this extended modeling language, users can develop, for instance, simulation programs that employ the data for improved accuracy, or develop simulation programs that generate data for more comprehensive data analysis. Because there are already notable productive tools and frameworks for data analysis, such as Hadoop and Spark, as well as

many kinds of machine learning frameworks available, our extension of the modeling language focuses on the area of connecting it to simulations, and providing a common runtime environment for different kinds of frameworks and simulators.



Developing an end-to-end solution from simulation modeling to data processing



Field Theory Research Team

Team Leader **Yoshinobu Kuramashi** kuramasi@riken.jp

Novel Approach to Studying Computational Sciences Employing Computational Elementary Particle Physics

Our research field is the physics of elementary particles and nuclei, which tries to answer questions as old as the history of mankind: What is the smallest component of matter, and what is matter's most fundamental interaction? This research subject is related to the early universe and nucleosynthesis resulting from the Big Bang. Another important focus of ours is quantum properties, which play an essential role in the world of elementary particles and nuclei, as well as in 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).

Successful numerical simulations heavily depend on raising computer performance by improving algorithms and computational techniques. However, that is a difficult challenge given the trend of computer architecture is to employ increasingly large-scale hierarchical parallel structures consisting of tens of thousands of nodes, which individually have increasing numbers of CPU cores and arithmetic accelerators with even higher degrees of parallelism. We need to develop new types of algorithms and computational techniques different from conventional types, to achieve better computer performance. We will overcome this difficult situation by collaborating with applied mathematicians and computer scientists.

Career of Team Leader

- 2010 Team Leader, Field Theory Research Team, AICS, RIKEN (-present)
- 2012 Professor, University of Tsukuba (-present)
- 2007 Associate Professor, University of Tsukuba
- 1995 D. Sci., The University of Tokyo

Publications

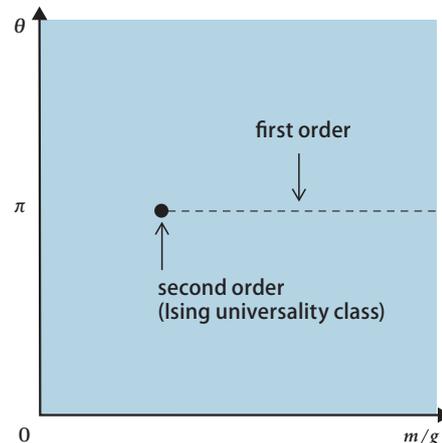
1. X.-Y. Jin, Y. Kuramashi, Y. Nakamura, S. Takeda, and A. Ukawa.: "Critical Point Phase Transition for Finite Temperature Three-Flavor QCD with Non-Perturbatively $O(a)$ -Improved Wilson Fermions at $N_t=10$," *Physical Review D* 96 (2017) 034523.
2. Y. Shimizu and Y. Kuramashi.: "Grassmann Tensor Renormalization Group Approach to One-Flavor Lattice Schwinger Model," *Physical Review D* 90 (2014) 014508.

Recent Achievement

Analyzing the phase structure of two-dimensional QED The Tensor Network (TN) scheme has been evolving conceptually and practically over the past fifteen years, and has produced theoretical and computational tools in various fields. In elementary particle physics, we recently succeeded in applying the Grassmann Tensor Renormalization Group (GTRG) algorithm, a TN scheme, to the analysis of the phase structure of one-flavor lattice Schwinger model (two-dimensional QED). The results show that the algorithm is free from the sign problem, and the computational cost is comparable to bosonic case, thanks to the direct manipulation of the Grassmann variables. This was the first successful application of a TN scheme to a Euclidean lattice gauge-theory including relativistic fermions.

Furthermore, we also performed analysis on the phase structure of the one-flavor lattice Schwinger model with the so-called θ -term. In spite of the complex action, we have succeeded in reproducing the phase structure predicted by analytical calculations. This provides evidence that the GTRG algorithm has the ability to treat complex actions. Our work has shown that the GTRG algorithm solves the notorious sign problem inherent in the Monte Carlo method by using the Schwinger model as a testing ground. Toward

the final goal of investigating four-dimensional lattice QCD, which is the $SU(3)$ non-Abelian gauge theory with relativistic fermions, we are currently studying higher dimensional models including non-Abelian gauge theories.



Phase diagram of one-flavor Schwinger model with θ -term



Discrete Event Simulation Research Team

Team Leader **Nobuyasu Ito** ito@ap.t.u-tokyo.ac.jp

Using Supercomputer Simulation Modeling to Study Non-continuous Phenomena

Supercomputers have been designed mainly for simulating partial and ordinary differential equations, but practical applications of such equations are limited. In a given system, it is quite common that something happens when a certain condition occurs, and something else happens when a different condition takes place. Vehicular-traffic simulations are a good example. A car stops at a red traffic signal, but continues driving when the signal is green; and the speed of a car may differ before and after passing through a crossing. Another example is disease propagation: an uninfected susceptible person may become infected after contracting a certain amount of pathogen. Such discrete-event research often requires enormous numbers of simulations depending on how many samples of event cascades and combinations are used.

We are investigating such discrete simulations using the K and post K supercomputers and statistical physics. Our current focus of research is on certain areas of social phenomena: traffic operations, economics activities and social relations. We have developed and made available to academic institutions an application software package named "OACIS" that can execute thousands to millions of simulations with appropriately selected input parameters, and which enables flexible analysis of their results. Users of OACIS are applying the software not only to social simulation events, but also to simulations in such fields as robotics and material design.

Career of Team Leader

- 2012 Team Leader, Discrete Event Simulation Research Team, AICS, RIKEN (-present)
- 1997 Associate Professor, Graduate School of Engineering, The University of Tokyo
- 1991 Researcher, Information Systems Center, Japan Atomic Energy Research Institute
- 1991 DSc, Graduate School of Science, The University of Tokyo

Publications

1. Y. Murase, T. Uchitane and N. Ito, "An open-source job management framework for parameter-space exploration: OACIS," Proceedings of the 30th Annual Workshop "Recent Developments in Computer Simulation Studies in Condensed Matter Physics" (The University of Georgia, Athens, U.S.A., February 20-24, 2017).
2. 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, 014801 (2017).
3. Takayuki Hiraoka, Takashi Shimada and Nobuyasu Ito, "Order-disorder transition in repulsive self-propelled particle systems," Phys. Rev. E vol.94 (2016) 062612.

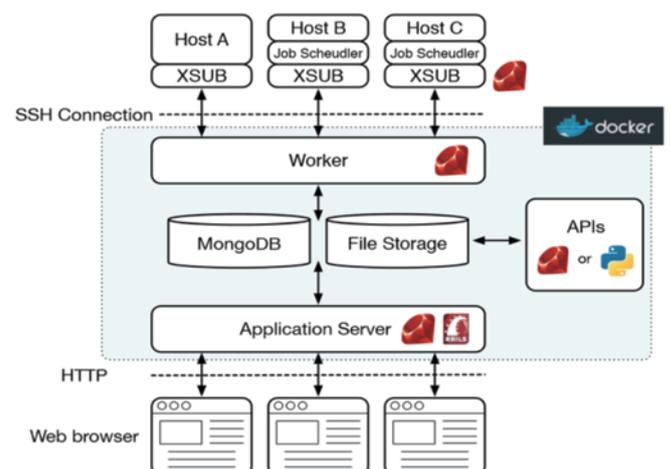
Recent Achievement

Development of simulation management applications Simulation studies often require the execution and analysis of an enormous number of simulations, which current massive-parallel supercomputers are capable of carrying out. However, designing and executing millions of different simulations are usually impractical. It is urgently necessary, therefore, to remove this obstacle in order to realize such studies, and this can be done by accelerating supercomputer applications.

Hence, we have developed OACIS, an open-source application software package, which we publicly released in 2014. Users operate OACIS through a web browser via a network. After installing OACIS on their computers, users upload and then register their own simulation and analysis software with OACIS together with specifies execution parameters. OACIS submits these jobs for execution via the network, monitors their status and gathers results when they are completed. APIs for Ruby and Python programs are available so that these programs can operate OACIS instead of the user.

In employing OACIS on the K and other supercomputers, we have studied various social simulations. Our results include the development of a simulation method to study important factors of

vehicular traffic in a city, and we have applied it to the city of Kobe's traffic system. We have also developed a method to study the bottleneck factor that arises when people flee from major disasters. This we have applied to evacuation planning in the event of a tsunami attack on the cities of Kanazawa and Kamakura.



Central dotted box shows structure of OACIS



Computational Molecular Science Research Team

Team Leader **Takahito Nakajima** nakajima@riken.jp

Team Website http://labs.aics.riken.jp/nakajimat_top/EHome.html

Development of a New Molecular Science Based on Original Theorizing and Use of K Computer-Compatible Software

We are chiefly interested in theoretical and computational molecular science based on quantum chemistry. Our main background is molecular orbital theory. In particular, we aim to develop interdisciplinary research that combines quantum chemistry with other research fields such as condensed matter physics and computer science. With the emergence of peta-scale computing platforms, we are entering a new period of modeling. Computer simulations of larger, more complicated, and more realistic systems than ever before can now be carried out. To benefit fully from the K computer, we are forging a new molecular science based on original theorizing and employment of our K computer-compatible software that can predict outcomes of molecular experiments.

In leading the way toward a new frontier of theoretical and computational molecular science, the project involves the novel development of theory, algorithms, and software, which will be realized through the collaborative use of the K computer across the fields of computational science and computer science. The specific topics involve: (1) Development of large-scale molecular theory to realize first-principles molecular calculations with tens of thousands of atoms. (2) Development of a highly-accurate molecular theory which is applicable to complicated molecular systems. (3) Development of relativistic molecular theory to accurately treat heavy-element molecular systems. (4) Development of a new program package for molecular theory: "NTChem". (5) Applications for molecular systems to clarify the mechanism of their chemical reaction and functionality.

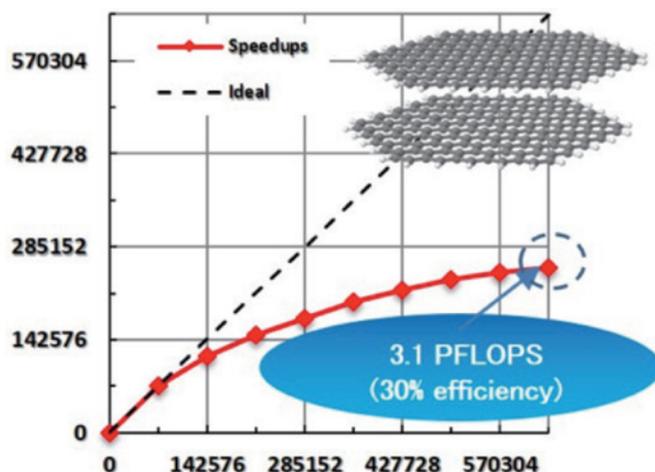
Recent Achievement

NTChem: A high-performance software package for quantum molecular simulation Quantum chemistry software comprises immensely useful tools for material and biological science research. Widely diverse programs have been developed in Western countries, but Japan has lagged behind. Our mission is to provide K computer users with 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. Therefore, we decided to develop NTChem: a comprehensive chemistry software package. NTChem is completely new and 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 NTChem are: ① electronic structure calculation of the ground state of molecules; ② linear-scaling DFT; ③ excited-state DFT calculation; ④ accurate electron correlation methods for ground and excited states; ⑤ massively parallel computing on the K computer and other architectures; ⑥ relativistic electronic structure calculation; ⑦ model calculations for large molecular

systems; ⑧ calculation of solvation effects; ⑨ efficient calculation for chemical reaction pathway; ⑩ ab initio molecular dynamics calculation; ⑪ calculation of electric and magnetic properties and ⑫ population analysis.



Parallel efficiency of the electron-correlation calculation with NTChem on the K computer

Career of Team Leader

- 2010 Team Leader, Computational Molecular Science Research Team, AICS, RIKEN (-present)
- 2009 Associate Team Leader, RIKEN
- 2004 Associate Professor, The University of Tokyo
- 2003 Lecturer, The University of Tokyo
- 1999 Research Associate, The University of Tokyo

Publications

1. T. Yonehara, T. Nakajima, "A quantum dynamics method for excited electrons in molecular aggregate system using a group diabatic Fock matrix", *J. Chem. Phys.* 147, 074110 (2017). <http://dx.doi.org/10.1063/1.4998746>.
2. R. Maitra, Y. Akinaga, T. Nakajima, "A coupled cluster theory with iterative inclusion of triple excitations and associated equation of motion formulation for excitation energy and ionization potential", *J. Chem. Phys.* 147, 074103 (2017). <http://dx.doi.org/10.1063/1.4985916>.
3. T. Nakajima, M. Katouda, M. Kamiya, Y. Nakatsuka, "NTChem: A high-performance software package for quantum molecular simulation", *Int. J. Quantum Chem.* 115, 349-359 (2015). DOI: 10.1002/qua.24860.



Computational Materials Science Research Team

Team Leader **Seiji Yunoki** yunoki@riken.jp

Developing Highly Efficient Simulations for Strongly Correlated Quantum Systems

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, which played a major role in the advance of today's 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.

Career of Team Leader

- 2010 Team leader, Computational Materials Science Research Team, AICS, RIKEN (-present)
- 2008 Associate Chief Scientist, Computational Condensed Matter Physics Laboratory, RIKEN
- 1996 Graduated from Applied Physics, Graduate School, Division of Engineering, Nagoya University

Publications

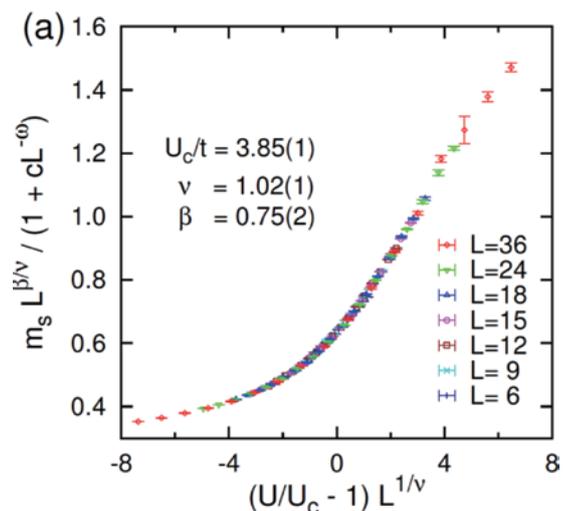
1. Y. Otsuka, S. Yunoki, and S. Sorella, "Universal quantum criticality in metal-insulator transition of two-dimensional interacting Dirac electrons", *Phys. Rev. X* 6, 011029 (2016).
2. S. Sota, S. Yunoki, and T. Tohyama, "Density-matrix renormalization group study of third harmonic generation in one-dimensional Mott insulator coupled with phonon", *J. Phys. Soc. Jpn.* 84, 054403 (2015).
3. S. Sorella, Y. Otsuka, and S. Yunoki, "Absence of a Spin Liquid Phase in the Hubbard Model on the Honeycomb Lattice", *Scientific Reports* 2, 992 (2012).

Recent Achievement

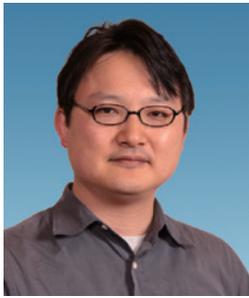
Largest simulations ever for interacting Dirac electrons and universality of metal-insulator transitions

Understanding the nature of metal-insulator transitions induced by Coulomb repulsion between electrons has been one of the most fundamental issues in condensed matter physics. Considering the simplest model, i.e., a Hubbard model on the honeycomb lattice, we have analyzed the metal-insulator transition that occurs in this model when increasing the repulsive interaction. This model has attracted lots of interests because it is considered as one of the most effective models for graphene, where the non-interacting electrons exhibit the relativistic Dirac dispersion.

We have developed a quantum Monte Carlo software application to perform the largest ever simulations for the Hubbard model, which were performed on the K computer. Our highly optimized software allows us to treat 2,592 electrons, which is four times larger than the previous world record (648 electrons). Most importantly, we have shown that there is no intermediate phase between the metallic and insulating phases, thus the transition is continuous. In addition, we have determined with high accuracy the critical exponents that characterize this metal-insulator transition of interacting Dirac electrons. In the future, we will attempt even larger simulations to address more fundamental issues in modern condensed matter physics, which, until now, have not been considered possible.



Metal-insulator transitions occurring for different system sizes (2L2) follow the universal function. The exponents (β and ν) in this function characterize the transitions.



Computational Biophysics Research Team

Team Leader **Yuji Sugita** sugita@riken.jp

Team Website <http://www.riken.jp/TMS2012/cbp/en/index.html>

Development of High-Performance Molecular Dynamics Simulation Methods for Biomolecular Structures and Functions

Proteins, nucleic acids, lipid molecules and other biomolecules play key roles in a cell's biological functions. Their atomistic structures are usually determined by experiments, using crystallography, nuclear magnetic resonance (NMR), and cryo-electron microscopy. It is also important to determine their conformational dynamics, for understanding the structure-dynamics-function relationship will help advance the life sciences and new drug discoveries. Molecular dynamics (MD) simulations of biomolecules are often used for this purpose, but they need to become much faster to overcome the current limitations in spatial and temporal scales.

We are developing a new MD simulation program: GENESIS (Generalized-Ensemble Simulation System) and improving its performance through optimization and parallelization. In addition, we are developing novel computational algorithms for modeling large-scale conformational changes of biomolecules, such as the replica-exchange method and the string method that connect between two structures. Multi-scale modeling techniques combining atomistic models, coarse-grained models, and hybrid quantum mechanics-molecular mechanics models are also necessary for our simulations.

Coupling between simulations and experiments is yet another important subject in computational biology. We are applying several data-analysis methods, data assimilation and machine learning to link single-molecule-measurement time-series with MD simulations of biomolecules.

Career of Team Leader

- 2010 Team Leader, Computational Biophysics Research Team, AICS, RIKEN (-present)
- 2002 Lecturer, Institute of Molecular and Cellular Biosciences, The University of Tokyo
- 1998 Research Associate, Institute for Molecular Science
- 1998 Ph. D (Chemistry), Graduate School of Science, Kyoto University

Publications

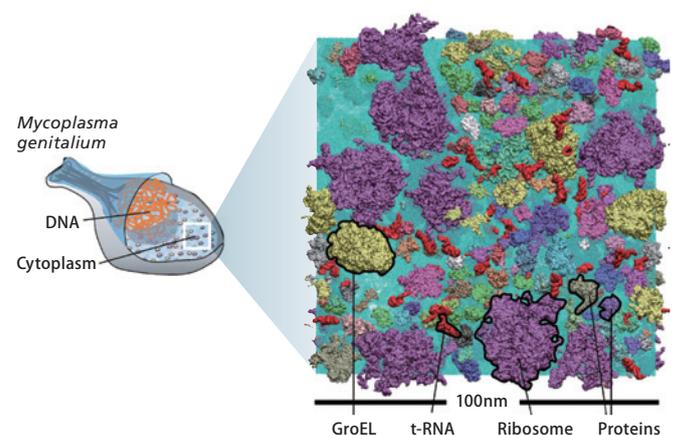
1. Biomolecular interactions modulate macromolecular structure and dynamics in atomistic model of a bacterial cytoplasm, Isseki Yu, Takaharu Mori, Tadashi Ando, Ryuhei Harada, Jaewoon Jung, Yuji Sugita, and Michael Feig, *eLife* 5, e19274 (2016).
2. GENESIS: A hybrid-parallel and multi-scale molecular dynamics simulator with enhanced sampling algorithms for biomolecular and cellular simulations, Jaewoon Jung, Takaharu Mori, Chigusa Kobayashi, Yasuhiro Matsunaga, Takao Yoda, Michael Feig, and Yuji Sugita, *WIREs Comp. Mol. Sci.* 5, 310-323 (2015).
3. Reduced Native State Stability in Crowded Cellular Environment Due to Protein-Protein Interactions, Ryuhei Harada, Naoya Tochio, Takanori Kigawa, Yuji Sugita, and Michael Feig, *J. Am. Chem. Soc.* 135, 3696-3701 (2013).

Recent Achievement

The first molecular dynamics simulations of an atomistic model of the bacteria cytoplasm Conformational dynamics of a protein or nucleic acid is often investigated with conventional MD simulations. In such an analysis, a single biomolecule is solvated in solvent water and is simulated as long as possible to examine the structure-dynamics-function relationship. As well as molecular interaction between biomolecules in cellular environments such as the cytoplasm, investigation of the biological membrane and cellular nuclei are also essential for understanding biological cellular functions. However, due to the limitations in computational resources and power of MD software, these studies have not been performed until now.

We have optimized and parallelized our MD software GENESIS for simulating large biological systems that contain more than 10 million atoms. *Mycoplasma genitalium* is one of the smallest bacteria whose genetic and proteomic information is abundant. Based on this information, an atomistic model of the bacteria cytoplasm with its many proteins, RNAs, ribosomes, ions, metabolites like ATP, and water molecules was built, and was then simulated using GENESIS on the K computer. The detailed trajectory analysis produced

new insights into protein stability, diffusion, and specific and non-specific interactions in the cytoplasmic environments. Biomolecular simulations in cellular environments are expected to contribute not only to the life sciences but also to new drug discoveries.



Computer simulation of an atomistic model of the bacteria cytoplasm



Particle Simulator Research Team

Team Leader **Junichiro Makino** jmakino@riken.jp

Team Website <http://www.jmlab.jp/?lang=en>

Framework for the Simplified Development of High-performance Particle-based Simulation Programs

Systems modeled in numerical simulations can be classified as regular grid, irregular grid, and particle systems. As the computational environment evolves, ever larger simulations have become possible. Thus, particle-based methods which can handle complex and dynamically changing shapes without special treatment, have become more important. However, it is a challenge to develop efficient parallel programs for particle-based simulations on large parallel systems such as the K or post-K computers. We need to efficiently implement domain decomposition with near-ideal load balancing, exchange particles between domains, and improve interaction calculations of particles in different domains. On the other hand, all parallel particle simulation-programs require these functions.

Consequently, we are developing the Framework for Developing Particle Simulators (FDPS), which can be used to produce any kind of particle-based simulation. FDPS receives particle data structures and functions, evaluates interactions between particles, and generates efficient libraries for parallelization. Thus, users of FDPS can develop their own highly efficient parallel particle simulation-programs without spending large amounts of time, and so can concentrate on realizing their goals.

Career of Team Leader

- 2016 Professor, Kobe University, Graduate School of Science, Department of Planetology (-present)
- 2014 Deputy Project Leader, AICS, REKEN, Flagship 2020 Project (-present)
- 2012 Team Leader, Particle Simulator Research Team, AICS, RIKEN (-present)
- 1990 Research Associate, The University of Tokyo, College of Arts and Sciences
- 1990 Ph.D, The University of Tokyo, Graduate School of Arts and Sciences

Publications

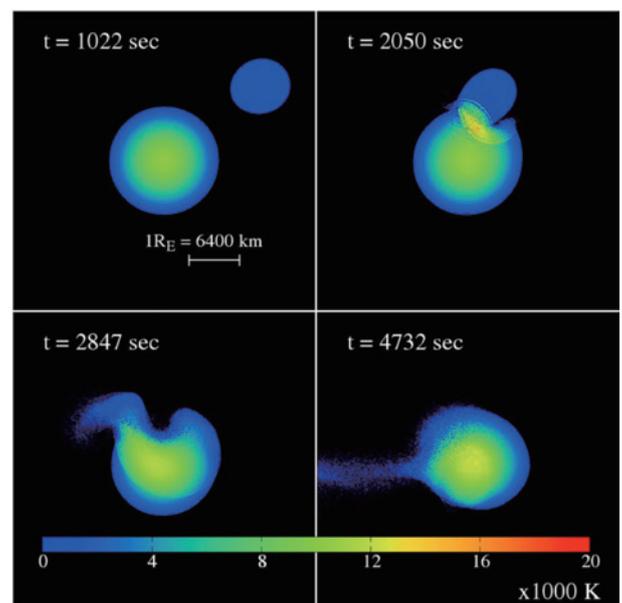
- Hosono, N., M. Iwasawa, A. Tanikawa, K. Nitadori, T. Muranushi, and J. Makino, Unconvergence of very-large-scale giant impact simulations, Publications of the Astronomical Society of Japan, 2017, 69, 26-.
- Iwasawa, M., A. Tanikawa, N. Hosono, K. Nitadori, T. Muranushi, and J. Makino, Implementation and performance of FDPS: a framework for developing parallel particle simulation codes, Publications of the Astronomical Society of Japan, 2016, 68, 54-.
- Iwasawa, M., S. Portegies Zwart, and J. Makino, GPU-enabled particle-particle particle-tree scheme for simulating dense stellar cluster system, Computational Astrophysics and Cosmology, 2015, 2, 6-.

Recent Achievement

World's first highly efficient general-purpose framework for particle-based simulations

By employing FDPS, we have succeeded in creating application programs for particle-based simulations not specifically optimized for large-scale parallel computing to run efficiently on top-ranked supercomputers such as the K computer. On the K computer, we achieved efficiency gains of around 50% for gravitational many-body simulations and for SPH simulations, at up to full-node execution. FDPS also supports GPGPU systems, and application programs can be developed both with C++ and the Fortran languages. We are currently working on a highly efficient implementation for heterogeneous many-core systems.

FDPS has already been used for various large-scale simulations, including the largest simulation ever of the giant impact hypothesis used to explain the moon's formation, and the first full simulation of rings around asteroids. These simulations would have been impossible without FDPS.



Largest simulation of the giant impact hypothesis used to explain the moon's formation



Computational Climate Science Research Team

Team Leader **Hirofumi Tomita** htomita@riken.jp

Team Website https://climate.aics.riken.jp/top_e.htm

Fundamental Study of Global-LES Simulations, with a Development of a Basic Library for Climate Science

Advanced supercomputers, including the K computer, make possible simulation of the global atmosphere by using a high-resolution global cloud-resolving model with a grid size of less than 1km. Since the global cloud-resolving model still cannot explicitly express sub-grid scale phenomena related to atmospheric small eddies and cloud generation, these phenomena are parameterized even in high-resolution models. The use of the parameterization scheme leads to uncertainty and/or bias in the simulated results. In the future, such uncertainty is expected to be reduced by using a global-LES (large eddy simulation) model relying on basic climate principles.

However, to realize global-LES simulations a number of challenges have to be overcome: understanding the spatial-resolution dependency of LES schemes, the development of a new theoretical basis of LES for real-atmosphere simulation, raising the sophistication level of physical process schemes, improving their computational performance, and preparation of a post-process library for analyzing a huge number of model outputs. To advance global-LES simulations, we will address several climate science targets: hierarchical structure of clouds, and exploration of multiple equilibrium solutions under ideal conditions, as well as regional climate studies under real atmospheric conditions.

Career of Team Leader

- 2011 Team Leader, Computational Climate Science Research Team, AICS, RIKEN (-present)
- 2007 Senior Scientist, Research Institute of Global Change, JAMSTEC (fka Frontier Research Center for Global Change)
- 1999 Researcher, Frontier Research Center for Global Change (fka Frontier Research System for Global Change)
- 1999 Graduated from Graduate school of engineering, The University of Tokyo

Publications

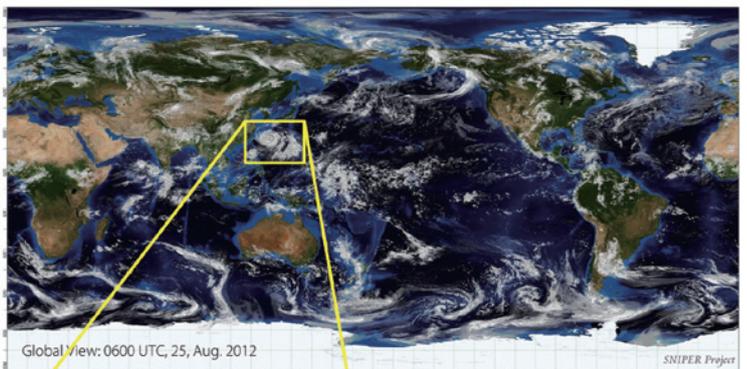
1. Yoshida, R., S. Nishizawa, H. Yashiro, S. A. Adachi, Y. Sato, T. Yamaura, and H. Tomita (2017): CONeP: A cost-effective online nesting procedure for regional atmospheric models, *Parallel Computing*, 65, 21-31, doi: 10.1016/j.parco.2017.04.004.
2. Nishizawa, S., H. Yashiro, Y. Sato, Y. Miyamoto, and H. Tomita, 2015, Influence of grid aspect ratio on planetary boundary layer turbulence in large-eddy simulations, *Geosci. Model Dev.*, 8, 3393-3419, doi:10.5194/gmd-8-3393-2015.
3. Miyamoto, Y. and Y. Kajikawa, R. Yoshida, T. Yamaura, H. Yashiro and H. Tomita (2013): Deep moist atmospheric convection in a sub-kilometer global simulation, *Geophys. Res. Lett.*, doi:10.1002/grl.50944.

Recent Achievement

Realistic expression of cumulonimbus clouds with a super-high-resolution simulation of the global atmosphere

The world's first simulation of the global atmosphere with a horizontal resolution less than 1 km was performed using a global cloud-resolving model. This exceedingly high-resolution experiment enabled clouds such as cumulonimbus to be resolved using several grid cells in the model. When the grid size was reduced to less than 2 km, expression of the simulated cumulonimbi were improved and resembled the observed clouds. In other words, the clouds were explicitly resolved in the model. To examine the convergence of results from simulations with different horizontal grid-sizes and to evaluate uncertainty in the conclusions, further studies using a LES model with finer spatial resolution will be required.

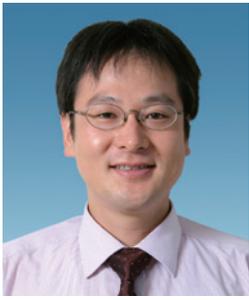
Grid spacing: 870m



Grid spacing: 3.5km (for comparison)



Global atmospheric simulation with a grid spacing of 870 meters



Complex Phenomena Unified Simulation Research Team

Team Leader **Makoto Tsubokura** mtsubo@riken.jp

Researching and Developing a Framework for Complex Phenomena Unified Simulations and Its Application to Industrial Problems

Most complex phenomena observed in manufacturing processes are relating to or coupled with other physical or chemical phenomenon such as turbulence diffusion, structure deformation, heat transfer, aeroacoustics, electromagnetic fields or chemical reactions. While the use of computer simulations is rapidly spreading in industry as a helpful engineering tool, its limitations regarding coupled phenomena is now well recognized. This is because each simulation method has been optimized for a specific phenomenon, and once two or more solvers of different phenomena are coupled to deal with a complicated target, computational performance is seriously degraded. Thus our main objective is to establish a new simulation framework for complex and coupled phenomena by utilizing the HPC environment and to expand its use in engineering applications by fostering next-generation digital engineering.

For that purpose, we are researching and developing a unified simulation method called CUBE. Its goal is to solve multiple partial differential equations on the same hierarchically structured grid system. To date, we have singled out three main areas to improve this method. First, to speed up CUBE by considering next-generation hardware architecture and to realize real time simulations for industrial use. Second, to improve the accuracy of CUBE for dealing with coupled phenomena when realizing real world simulations for engineering applications, as this will expand the possibility of using simulations in real operating conditions. Third, to promote the sophisticated use of CUBE in manufacturing processes: For example, applying it to multi-objective optimization by utilizing assimilation of existing experimental data, or by applying deep learning to big data simulations.

Career of Team Leader

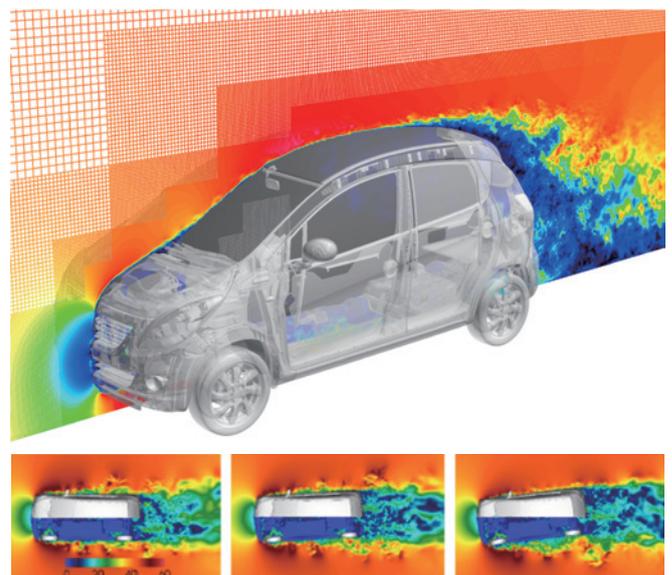
- 2015 Professor, Graduate School of System Informatics, Kobe University (-present)
- 2012 Team Leader, Complex Phenomena Unified Simulation Research Team, AICS, RIKEN (-present)
- 2007 Associate Professor, Faculty of Engineering, Hokkaido University
- 1997 Ph.D, Faculty of Engineering, The University of Tokyo

Publications

1. Chung-Gang Li, Makoto Tsubokura: An implicit turbulence model for low-Mach Roe scheme using truncated Navier-Stokes equations, *Journal of Computational Physics*, vol.345, pp.462-474, DOI: 10.1016/j.jcp.2017.05.032 (2017)
2. Chung-Gang Li, Makoto Tsubokura, Rahul Bale: Framework for simulating natural convection in practical applications, *International Communication in Heat and Mass Transfer*, vol.75, pp.52-58, DOI: 10.1016/j.icheatmasstransfer.2016.03.022 (2016)
3. Keiji Onishi, Makoto Tsubokura: Vehicle Aerodynamics Simulation for the Next Generation on the K computer: Part 2 Use of Dirty CAD Data with Modified Cartesian Grid Approach, *SAE International Journal of Passenger Cars - Mechanical Systems*, 7(2): 2014-01-0580(2014)

Recent Achievement

Simulation of a Vehicle's Coupled Aerodynamics and 6DoF-Motion in Real Driving Conditions By developing a new hybrid Euler-Lagrangean moving boundary method for the immersed boundary technique, and implementing it in the CUBE unified simulation framework, we have made it possible to simulate vehicular aerodynamics coupled with 6DoF motion. We successfully conducted a real-world simulation of a vehicle in cornering conditions. To achieve this, we used both detailed and dirty CAD data (provided by an automotive OEM) and the wheel rotation together with the front wheels' steering angle-change in order to reproduce the vehicle's complicated shape. This innovative simulation makes it possible to evaluate high-speed drivability from CAD data only. This presents new manufacturing possibilities for vehicle makers by means of optimizing a vehicle's total performance in an integrated manner at an early stage of development before real prototyping begins.



Simulation of coupled vehicle aerodynamics and 6DoF-motion utilizing CUBE



HPC Programming Framework Research Team

Team Leader **Naoya Maruyama** nmaruyama@riken.jp

Programming Models for Large-Scale High Performance Computing Systems

We develop high performance, highly productive software stacks that aim to simplify development of optimized, fault-tolerant supercomputer applications for computational science. Our focus includes large-scale data processing, heterogeneous computing, and fault tolerance systems. We are developing 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 of our projects focuses on increasing performance and productivity in large-scale heterogeneous systems. We are also investigating high performance graph analytics on the K computer. In particular, our work on the Graph500 benchmark has already allowed us to obtain the highest performance in the world using the K computer.

Career of Team Leader

- 2012 Team Leader, HPC Programming Framework Research Team, AICS, RIKEN (-present)
- 2009 Assistant Professor, Tokyo Institute of Technology
- 2008 Postdoctoral Researcher, Tokyo Institute of Technology
- 2008 PhD, Tokyo Institute of Technology

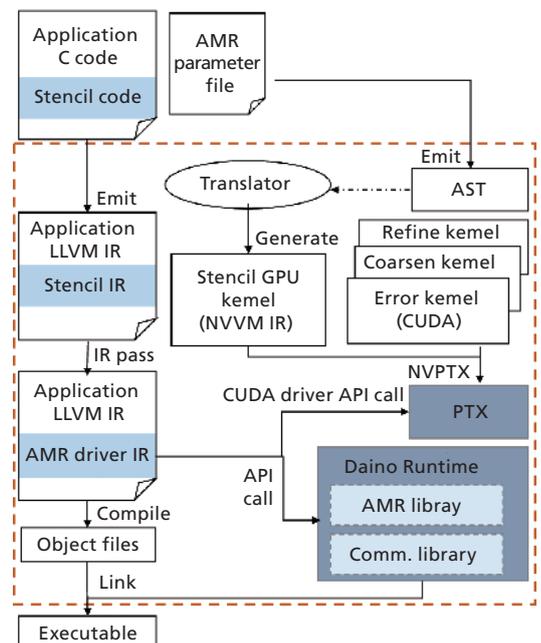
Publications

1. Koji Ueno, Toyotaro Suzumura, Naoya Maruyama, Katsuki Fujisawa, and Satoshi Matsuoka, "Efficient Breadth-First Search on Massively Parallel and Distributed-Memory Machines," Data Science and Engineering, vol. 2, pp. 22-35, 2017.
2. Mohamed Wahib, Naoya Maruyama, and Takayuki Aoki, "Daino: a high-level framework for parallel and efficient AMR on GPUs," ACM/IEEE SC'16, 2016. (Best Paper Award)
3. Hamid Reza Zohouri, Naoya Maruyama, Aaron Smith, Motohiko Matsuda, and Satoshi Matsuoka, "Evaluating and optimizing OpenCL kernels for high performance computing with FPGAs," ACM/IEEE SC'16, 2016.

Recent Achievement

Simplifying Development of Applications for Supercomputers As part of our research on application frameworks, we have developed a framework for computational fluid dynamics applications using the Adaptive Mesh Refinement (AMR) algorithm. AMR allows for significant reduction of both compute and memory requirements by adaptively managing mesh granularity of a given simulation domain; however, in reality, due to its complexity in dynamically changing mesh granularity, it has only been employed in a very limited set of relatively small-scale applications.

This problem is particularly challenging in heterogeneous systems with GPU accelerators since the overhead of data movement is much greater. To solve the problem, we have developed the Daino framework, which allows the user to develop high-performance AMR applications in a simple manner. The framework extends an existing standard compiler and aggressively applies automated program-transformation techniques for optimizing user applications for target architectures such as GPUs. As a result, an application developed using Daino is portable in both functionality and performance, as the automated translation of user code ensures that the application runs on different parallel systems efficiently without target-specific manual optimization. Our results demonstrated that an approach based on high-level frameworks such as Daino can achieve both high performance and high productivity even with complex large-scale systems such as supercomputers using GPU accelerators.



Overview of the Daino framework [Wahib2016]



Data Assimilation Research Team

Team Leader Takemasa Miyoshi takemasa.miyoshi@riken.jp

Team Website http://www.data-assimilation.riken.jp/index_e.html

Data Science Integrating Computer Simulations with Real-world Data

Data assimilation (DA) is a cross-disciplinary science to synergize computer simulations and real-world data, based on statistical mathematics and dynamical systems theory. As computer technology advances and enables precise simulations, it will become more important to compare simulations with real-world data.

We are researching and developing advanced DA methods and their various applications, and we aim to integrate computer simulations and real-world data in the most effective way. Particularly, we tackle the challenging problems involved in developing efficient and accurate DA systems for “big simulations” with real-world big data from various sources including advanced sensors. Our specific foci include 1) theoretical and algorithmic developments for efficient and accurate DA; 2) development of DA methods and applications by taking advantage of the world-leading K computer and big data derived from advanced new sensors; and 3) the exploration of new DA applications in wider simulation fields. These advanced DA studies will enhance simulation capabilities and lead to better use of high-performance computers including the K computer.

Career of Team Leader

- 2012 Team Leader, Data Assimilation Research Team, AICS, RIKEN (-present)
- 2011 Assistant Professor, University of Maryland, College Park, Maryland, USA
- 2005 Ph.D. in Meteorology, University of Maryland, College Park, Maryland, USA
- 2000 Technical Official, Planning Division, Japan Meteorological Agency

Publications

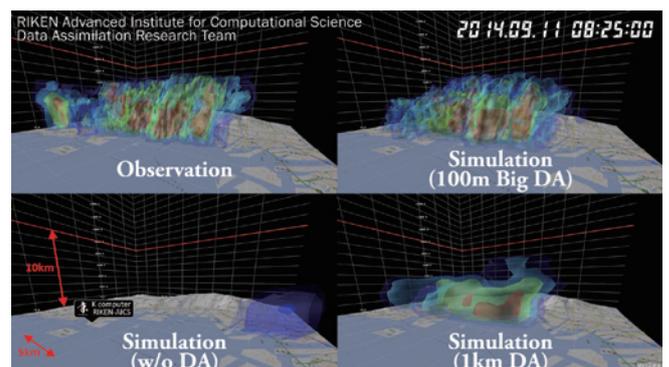
1. Miyoshi, T., G.-Y. Lien, S. Satoh, T. Ushio, K. Bessho, H. Tomita, S. Nishizawa, R. Yoshida, S. A. Adachi, J. Liao, B. Gerofi, Y. Ishikawa, M. Kunii, J. Ruiz, Y. Maejima, S. Otsuka, M. Otsuka, K. Okamoto, and H. Seko, 2016: "Big Data Assimilation" toward Post-peta-scale Severe Weather Prediction: An Overview and Progress. Proc. of the IEEE, 104, 2155-2179. doi:10.1109/JPROC.2016.2602560
2. Miyoshi, T., M. Kunii, J. Ruiz, G.-Y. Lien, S. Satoh, T. Ushio, K. Bessho, H. Seko, H. Tomita, and Y. Ishikawa, 2016: "Big Data Assimilation" Revolutionizing Severe Weather Prediction. Bull. Amer. Meteor. Soc., 97, 1347-1354. doi:10.1175/BAMS-D-15-00144.1
3. Miyoshi, T., K. Kondo, and K. Terasaki, 2015: Big Ensemble Data Assimilation in Numerical Weather Prediction. Computer, 48, 15-21. doi:10.1109/MC.2015.332

Recent Achievement

K computer and advanced weather radar come together to predict sudden torrential rains Using the K computer, we carried out 100 parallel simulations of a convective weather system, using the nonhydrostatic mesoscale model with 100-meter grid spacing and assimilated data from a next-generation phased-array weather radar, which was implemented in the summer of 2012 by the National Institute of Information and Communications Technology (NICT) and Osaka University. This enabled us to produce a high-resolution three-dimensional distribution map of rain every 30 seconds—120 times more rapidly than the typical hourly updated systems operated at weather prediction centers around the world today.

To test the accuracy of the system, we attempted to model a real case—a sudden storm that took place on September 11, 2014, in Kobe. The simulations were tested without observational data input, as well as with observational data incorporated every 30 seconds on 100-meter and 1-kilometer grid scales. The simulations alone were unable to replicate the rain, while the simulation incorporating observational data enabled the computer to represent the actual storm. In particular, the simulation carried out with 100-meter grids produced an accurate replication of the storm when com-

pared to actual observations.



Distribution of thunderclouds on September 11, 2014



Computational Disaster Mitigation and Reduction Research Unit

Unit Leader **Satoru Oishi** satoru.oishi@riken.jp

Unit Website http://bosai.riken.jp/index_en.html

Development of Large-scale Numerical Simulations of Multi-hazard Natural Disasters

We aim to develop and conduct large-scale numerical simulations of multi-hazard natural disasters, including earthquakes, tsunami, floods, landslides and mud slides.

Simulation of a natural disaster that can devastate an existing city requires the representation of existing buildings and infrastructures as equations and numerical data. These equations and data are defined as numerical city structure models. Cities have many kinds of structures. They are made up of, not only buildings whose design drawings are available, but also, for example, subway systems, domestic water and sewage pipes, and artificial river banks. We are developing cutting edge technology to represent these complex city components in numerical simulations.

We also aim to create large-scale numerical simulations of geotechnical hazards like liquefaction and slope failure because the underground conditions that produce such hazards is not well understood. We have developed efficient and manageable numerical methods to help us simulate such geotechnical hazards.

By combining these advanced simulations with seismic simulations and meteorological simulations, we aim to produce multi hazard simulations. We believe our research results will benefit citizens and governments alike, and will help create resilient societies.

Career of Unit Leader

- 2017 Unit Leader, Computational Disaster Mitigation and Reduction Research Unit, AICS, RIKEN (-present)
- 2009 Professor, Kobe University
- 2000 Associate Professor, University of Yamanashi
- 1998 Dr. Eng. Kyoto University
- 1993 Master Eng. Graduate School of Engineering Kyoto University

Publications

1. Chen, J., Supprasert, S., O-tani, H., Fujita, K., Wijerathne, L. and Hori, M.: "On elastic waves in granular assemblies: from a continuumization viewpoint," *Mechanics of Materials*, 109, 101-113, (2017).
2. Hori, M., Wijerathne, L., Chen, J. and Ichimura, T.: "Continuumization of Regularly Arranged Rigid Bodies," *Journal of JSCE*, 4(1), 38-45, (2016).
3. Chen, J., Takeyama, T., O-tani, H., Fujita, K. and Hori, M.: "A Framework for Assessing Liquefaction Hazard for Urban Areas Based on Soil Dynamics", *International Journal of Computational Methods*, 13, 1641011, (2016).

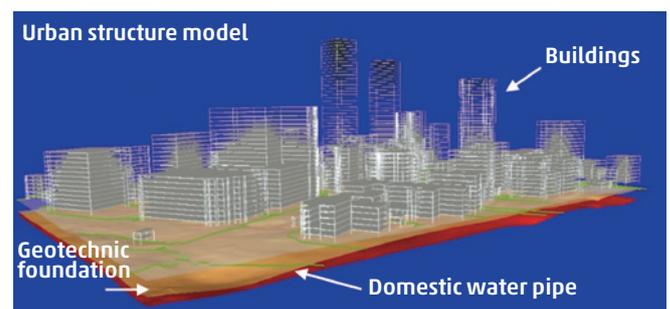
Recent Achievement

Hazard map based on large-scale simulations We have developed a next-generation hazard map depicting a possible scenario resulting from the predicted Nankai Trough Earthquake. Using large-scale numerical simulations, it includes four cities in Hyogo prefecture.

Previously, hazard maps were made from the results of simpler numerical simulations and empirical equations based on distribution of ground motion index values. However, the latest simulations using the K computer for next-generation hazard maps simulate propagation and amplification of seismic waves, and then calculate their physical impact on buildings. In other words, the latest simulations explicitly calculate the fragility curve. This calculation is an essential component for estimating damage to cities from earthquakes because the simulation includes the elemental physical process of the propagation of waves and the response of buildings to these waves.

Our numerical simulation developed to create next-generation hazard maps has two advanced features. The first is the comprehensive simulation of an entire city 100km² in area. Comprehensive simulation means both geotechnical wave propagation and urban

structures have been simulated simultaneously. This large-scale comprehensive calculation is performed on the K computer. This achievement resulted in the technology being chosen as a finalist for the Gordon Bell Prize. The second feature enables the technology to represent existing buildings in numerical simulations as data and equations. By using newly developed automated translation techniques, hundreds of thousands of buildings can be represented in such simulations.



Numerical city structure model



Computational Structural Biology Research Unit

Unit Leader **Florence Tama** florence.tama@riken.jp

Developing New Methods and Computational Tools for Integrative Structural Biology

Biomolecules such as proteins and RNA form large complexes that work together to accomplish core biological functions. Dysfunction of those biomolecules may result in severe diseases. To understand such diseases and develop treatments, mechanisms of these protein functions need to be understood. This requires determining their 3-dimensional structures. However, most biomolecules move and change their shapes upon accomplishing their functions, and such dynamic factors should also be considered.

3D structures of biomolecules are obtained primarily through experimental studies. For example, X-ray crystallography provides high-resolution structures. However, it requires crystallization of the biological molecule, which can be quite a challenge. In other methods, such as cryo-electron microscopy (cryo-EM), 2D images of the individual biological molecules are collected, and then be reassembled to form a 3D structure, though generally of a lower resolution. Still, this presents some advantages over X-ray crystallography as large complexes can be studied as well as their dynamics.

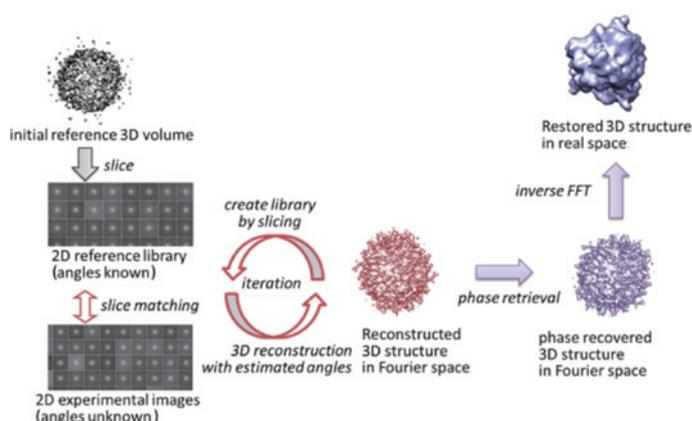
Recently, the X-ray free electron laser (XFEL) also opened the possibility to directly image single molecules, using its high intensity X-ray laser. Our interdisciplinary research unit aims to develop computational tools to determine 3D structures and dynamics, utilizing cryo-EM and XFEL experimental data. Such computational tools will be employed on the K and post-K computers to take advantage of the resources for large scale data analyses, and also to share these tools with the scientific community. Applications could provide new insights into the structure and dynamics of important biomolecules that are unattainable with existing techniques.

Recent Achievement

Restoring 3D structures from XFEL diffraction data Recent development of intense XFEL light sources offers the possibility to obtain new structural information of biological macromolecules, in particular imaging of single macromolecules. Atomic level resolution such as obtained by X-ray crystallography cannot yet be achieved given current experimental conditions. But as XFEL experiments are still undergoing development for routine applications, computational algorithms to understand and analyze experimental data also need to be developed. In particular, to restore the 3D structures of biomolecules from the 2D diffraction patterns obtained by XFEL experiments, computational algorithms are necessary to estimate the laser beam incidence-angles to the molecule.

We are working on a program package for XFEL analysis that is based on XMIPP, commonly used software 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 routines were modified to handle 2D data in Fourier space. Through an iterative procedure, the orientations of the biomolecules that each image represents are estimated, and the 3D structure factor-amplitude is reconstructed. The 3D model in real space is obtained by

phase retrieval. This approach was successfully tested with experimental data similar to XFEL diffraction patterns taken from a single nanoparticle.



3D structure restoring process

Career of Unit Leader

- 2015 Professor, Graduate School of Science, Nagoya University(-present)
- 2013 Unit Leader, Computational Structural Biology Research Unit, AICS, RIKEN(-present)
- 2006 Assistant Professor, University of Arizona, USA
- 2001 Post-doctoral researcher, The Scripps Research Institute, USA
- 2000 Ph.D. in Computational Biophysics, University Paul Sabatier, France

Publications

1. M. Nakano, O. Miyashita, S. Jonic, C. Song, D. Nam, Y. Joti and F. Tama. "Three-dimensional reconstruction for coherent diffraction patterns obtained by XFEL". *J. Synchrotron Rad.* 2017
2. O. Miyashita, C. Kobayashi, T. Mori, Y. Sugita, F. Tama. "Flexible Fitting to Cryo-EM Density Map using Ensemble Molecular Dynamics Simulations". *J. Comp. Chem.* 2017
3. A. Tokuhisa, S. Jonic; F. Tama and O. Miyashita. "Hybrid Approach for Structural Modeling of Biological Systems from X-ray Free Electron Laser Diffraction Patterns". *J. Struct. Biol.* 2016

Development of Human Resources

RIKEN Advanced Institute for Computational Science (AICS) plays a central role in the development of computational science and technology in Japan. AICS also actively utilizes the advanced technologies and knowledge accumulated through these activities and cooperates with related institutions to develop the personnel who will support computational science and technology.

RIKEN AICS conducts training for graduate students, young researchers and corporate engineers, aiming to develop:

- **Human resources who can coordinate and integrate computational and computer sciences**
- **Human resources with advanced computational science technology skills**
- **Human resources who will contribute to the promotion of the use of advanced computational science technologies in industry**

AICS Schools and Workshops

AICS offers school programs in computer programming and other subjects that include practical training, as well as workshops that are designed to encourage interchange among diverse research fields related to computational and computer

sciences and international exchanges. These programs and workshops are held for students, young researchers and other trainees.

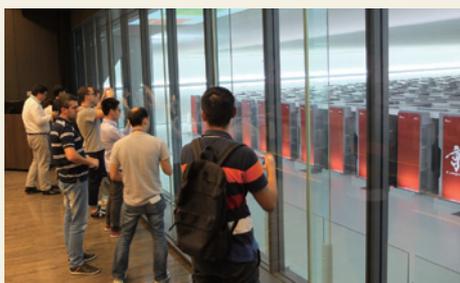
RIKEN AICS International HPC (High Performance Computing) Computational Science Internship Program (applications accepted in February - March, program held in June - October) *¹

This program for PhD holders affiliated with overseas institutions has been offered since FY 2017. Training is conducted for one to three months, usually between June and October.



RIKEN AICS HPC Computational Science Internship Program (applications accepted in May - June, program held in August - September) *²

This is a program for technical college students and university graduate students who live in Japan. Training is conducted for two weeks to a month, usually between August and September.



RIKEN AICS HPC Youth Workshop (applications accepted in December - January, program held in February) *¹

This program for students and young researchers has been offered since FY 2016. Through English presentations and discussions, the three-day workshop aims to create a network of collaborations among young researchers, and to foster their research communication and presentation skills in an international setting. Young researchers at overseas institutions that have ties to AICS also participate in the program.



SPRING

International HPC Summer School (applications accepted in January - February, program held in June) *¹

This five-day program is held jointly by institutions in Japan (AICS), Europe, the United States and Canada, usually in June. Through lectures and practical training conducted by leading researchers in the HPC-related fields, the trainees acquire new knowledge from a wide-ranging perspective and are able to experience international and cross-sectoral exchanges with other trainees of the same generation.



RIKEN AICS HPC Summer School (applications accepted in January - March, program held in June) *¹

This program for graduate students and PhD holders will be offered starting in FY 2018. The four and a half day program provides instruction in state-of-the-art research in computational science and technology fields, and also includes practical training. Young researchers at overseas institutions that have ties to AICS also participate in the program.



KOBE HPC Summer School (applications accepted in June - July, program held in August) *²

In this five-day school program, which is usually held in August, students and young researchers learn about the basics of programming techniques for mastering the use of parallel computers. In addition to lectures that include practical training, the program also features presentations by researchers on practical examples of the use of the K Computer as well as visits to the K Computer and the AICS facility.



SUMMER

AUTUMN

KOBE HPC Spring School (applications accepted in December - February, program held in March) *²

This school program teaches the basics of parallel computing and the programming skills needed to master the use of parallel computers (parallel computer programming). The three-day program is usually held in March. In contrast to the summer school which focuses on basic content, the spring school provides intermediate training.



WINTER

Note: Application and program periods in parentheses are a general guide; see the AICS website for specific information about the programs for each year.

*¹ Language: English *² Language: Japanese

Internship Programs

AICS accepts interns for the purpose of fostering the young researchers who will be the future leaders of HPC technologies and computational science. Through practical training and experience gained by working in AICS research teams, the trainees deepen their understanding of computer science technology and gain the ability to conduct state-of-the-art computational science research and development.

Programs

- International internship program: Doctorate holders affiliated with overseas institutions
- Internship program: Japanese technical college students and university graduate students (including foreign students)



Training Period

- RIKEN AICS International HPC Computational Science Internship Program: Training for one to three months, usually between June and October
- RIKEN AICS HPC Computational Science Internship Program: Training for 2 weeks to one month, usually between August and September



RIKEN Graduate Student and Researcher Programs

RIKEN has various programs that are designed to nurture the capabilities of young researchers. The two programs for students are the Junior Research Associate (JRA) program and the International Program Associate (IPA). There is also a Special Postdoctoral Researchers (SPDR) Program for young researchers.

Programs for Junior Scientists

■ JRA Program

This program provides part-time positions at RIKEN for those enrolled in Japanese university PhD programs to conduct research under the instruction of RIKEN scientists as Junior Research Associates (JRAs).

■ IPA Program

This program provides an opportunity for International Program Associates (IPAs) to conduct research at RIKEN under the supervision of RIKEN scientists as part of their work toward obtaining a PhD. IPAs are non-Japanese doctoral candidates, attending a Japanese or overseas graduate school participating in RIKEN's joint graduate program, and RIKEN provides them with a daily living allowance and may cover their housing costs for up to a maximum of three years while they are at RIKEN.

■ SPDR Program

This program provides a venue for creative researchers that received their PhD within the past five years to pursue independent research for a period of three years. RIKEN provides a vibrant research environment for young researchers of different nationalities that wish to actively pursue their research in the global arena.

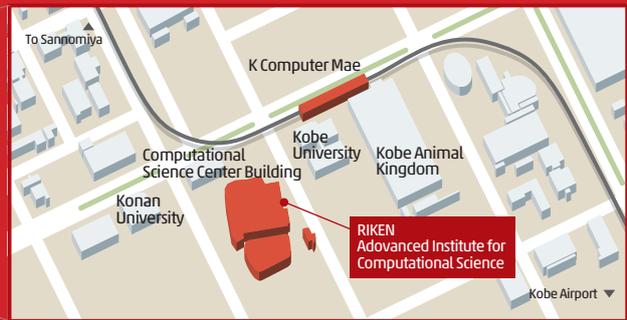
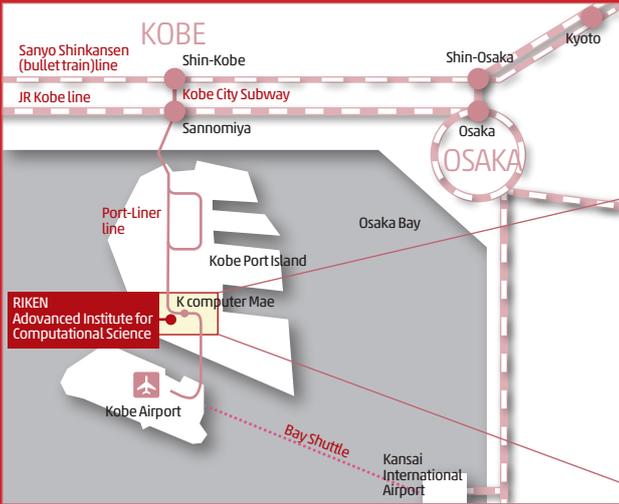
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