The Sixth
AICS International Symposium

Plans and future for international collaborations on extreme scale computing

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The Sixth AICS International Symposium

Plans and future for international collaborations on extreme scale computing

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Program

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Poster Session Program

Talk Session

(Day 1)

Monday, February 22

Overview of RIKEN AICS and International Collaborations in 2015/2016

Akira Ukawa[1]
[1] *Deputy Director and Head of Research Division, RIKEN AICS, Kobe, Japan*

Abstract

This talk serves as introduction to this year's AICS International Symposium which focuses on international collaboration toward extreme scale computing. A brief description is given of RIKEN AICS, including its missions, chronology, organization and recent research activities. This is followed by an overview of international collaborations conducted by AICS in recent years, and a discussion on possible future directions.

Biography

Akira Ukawa's field of expertize is theoretical particle physics, in particular large-scale numerical studies of lattice Quantum Chromodynamics. He is one of the pioneers of this field in which he has published over 300 articles and conference papers. He has also been deeply involved in research and development of parallel supercomputers for computational science in Japan, including the CP-PACS Project (1992-1996), which was ranked No. 1 in the Top 500 List in November 1996, and the PACS-CS Project (2005-2007), both at University of Tsukuba, the K computer Project (2006-2012), and most recently the post K computer Project. He has been dedicating his effort to interdisciplinary fusion between computational science and computer science.

The Convergence of HPC and Big Data

Pete Beckman[1]
[1] *Argonne National Laboratory, Argonne, IL, USA*

Abstract

For decades, the basic architecture of extreme-scale systems has been largely static. Our system architecture diagrams show compute nodes on the left, and big file systems on the right. On the left, we run a queuing system where jobs wait for hours or days. When they finally do run, they get MPI and a diskless nodes. On the righthand side we run a large shared Posix filesystem. This arrangement is out of step both with future architectures that provide NVRAM everywhere, advanced workflows, scientific databases, and in-situ data analysis. HPC must adopt a new, more agile system software architecture that can provide services to both HPC and Big Data computation. From the low-level operating system, such as the DOE Argo project, to the high-level workflow tools, we must bring together the two communities.

Biography

Pete Beckman is the co-director of the Northwestern University and Argonne National Laboratory Institute of Science and Engineering (http://naise.northwestern.edu) and is a recognized global expert in high-end computing systems. He designs software and hardware architectures for the world's largest supercomputers and leads the extreme-computing strategy at Argonne National Laboratory (http://www.anl.gov). Pete joined Argonne in 2002, serving first as director of engineering and later as chief architect for the TeraGrid, where he led the design and deployment team that created the world's most powerful Grid computing system for linking production HPC computing centers for the National Science Foundation. From 2008 to 2010 he was the director of the Argonne Leadership Computing Facility, where he led the Argonne team working with IBM on the design of Mira, a 10-petaflop Blue Gene/Q. Pete also coordinates the collaborative research activities in extreme-scale computing between the US Department of Energy and Japan's ministry of education, science, and technology. He leads a new project called Waggle (http://www.wa8.gl) to build intelligent attentive sensors. The Waggle technology and software framework is being used by the Chicago Array of Things (https://arrayofthings.github.io) project to deploy 500 sensors on the streets of Chicago beginning in 2016. Dr Beckman has a Ph.D. in computer science from Indiana University (1993) and a B.A. in computer science, physics, and mathematics from Anderson University (1985). In 2014, he received a Career Achievement Award from the Indiana University School of Informatics and Computing.

Development of system software stack for post K computer

Yutaka Ishikawa[1]
[1]*RIKEN AICS, Kobe, Japan*

Abstract

The next flagship supercomputer in Japan, replacement of K supercomputer, is being designed toward general operation in 2020. Compute nodes, based on a manycore architecture, connected by a 6-D mesh/torus network is considered. A three level hierarchical storage system is taken into account. A heterogeneous operating system, Linux and a light-weight kernel, is employed to build suitable environments for applications. In order to make maximum utilization of compute and storage resources, a system software stack, including communication and file I/O libraries on top of the heterogeneous operating system, is being designed. After brief introduction of the post K computer architecture, the design issues of the system software stack and current research and development activities will be presented.

Biography

Yutaka Ishikawa is the project leader of FLAGSHIP 2020 project at Riken AICS. Ishikawa received the BS, MS, and PhD degrees in electrical engineering from Keio University. From 1987 to 2001, he was a member of AIST (former Electrotechnical Laboratory), METI. From 1993 to 2001, he was the chief of Parallel and Distributed System Software Laboratory at Real World Computing Partnership. From 2002 to 2014, he was a professor at the University of Tokyo. He led development of cluster system software called SCore from 1993 to 2001, which was used in several large PC cluster systems around 2004. From 2006 to 2008, he led a project with other colleagues to design a commodity-based supercomputer called T2K open supercomputer. As a result, three universities, Tsukuba, Tokyo, and Kyoto, acquired each supercomputer based on the specification.

Collaborative Research between DoE Labs and Tokyo Tech GSIC on Extreme Scale Computing – Success Stories

Satoshi Matsuoka[1]
[1] *GSIC, Tokyo Institute of Technology, Tokyo, Japan*

Abstract

For modern-day science, no one country can fund all the technologies nor projects, and sharing of knowledge and efforts via international collaboration is a mandate. Tokyo Tech GSIC has been successfully pursuing international collaborations with top-tier HPC research institutions globally, in particular DoE labs such as Livermore, Oak Ridge, and Argonne, achieving tangible research results that saw publications in top-tier conferences and journals, with important topics such as resilience, performance modeling and visualization, detailed analysis of thread/cache/MPI interactions in hybrid codes, OpenACC extensions for GPU programming, and recently, graph processing frameworks on large machines equipped with NVMs. To make such collaborations successful, Ph.D. students are sent multiple times to the partner institutions to focus on a particular research topic with the researchers on site, sometimes leading to eventual DoE hiring. Such collaborations with physical presence of people over long term from Japan to US or vice versa, should be widened and funded at an increased level, for the advances of the entire HPC community.

Biography

Satoshi Matsuoka is a Full Professor at the Global Scientific Information and Computing Center (GSIC), Tokyo Institute of Technology. He is the leader of the TSUBAME supercomputers, including TSUBAME2.0, the first supercomputer in Japan to exceed Petaflop performance. He is also currently leading several major supercomputing research projects, such as the MEXT Green Supercomputing, JSPS Billion-Scale Supercomputer Resilience, as well as the JST-CREST Extreme Big Data. He has chaired numerous ACM/IEEE conferences including the ACM/IEEE Supercomputing Conference (SC13), and most recently won the 2014 IEEE-CS Sidney Fernbach Memorial Award, one of the most prestigious award in HPC.

Measuring and Analyzing an Entire HPC Center: The Sonar Project at LLNL

Todd Gamblin[1]
[1]*Lawrence Livermore National Laboratory, Livermore, CA, USA*

Abstract

As the complexity of HPC software and systems increases, performance variability is becoming an obstacle to understanding the throughput of supercomputers. Two runs of the same code, with the same input, may yield very different runtimes depending on compiler flags, system noise, dynamic scheduling, and shared system resources. Understanding an application's performance characteristics requires a large number of trial runs and measurements. Performance analysis has become a data-intensive task. To aid performance analysis, Livermore Computing has deployed Sonar, a "big data" cluster that will continuously collect and analyze performance data from our compute center. Sonar aggregates measurements from the network, file system, cluster nodes, applications, and facility. We describe how our tools integrate with Sonar, and we discuss some early techniques for predicting system performance data with Sonar.

Sonar represents of several steps towards increased automation at Livermore Computing. LLNL is also beginning to automate the deployment of tools and applications using a package manager called Spack. We give a brief overview of Spacks use at Livermore Computing, and how it can be used to apply performance tools to complex HPC applications.

Biography

Todd Gamblin is a Computer Scientist in the Center for Applied Scientific Computing at Lawrence Livermore National Laboratory. His research focuses on scalable tools and algorithms for measuring, analyzing, and visualizing the performance of massively parallel applications. He works closely with the Livermore Computing center and LLNL simulation code teams to build tools that allow users to deploy, run, debug, and optimize their software on machines with million-way concurrency.

Todd has been at LLNL since 2008. He received the Ph.D. and M.S. degrees in Computer Science from the University of North Carolina at Chapel Hill in 2009 and 2005. He received his B.A. in Computer Science and Japanese from Williams College in 2002. He has also worked as a software developer in Tokyo and held graduate research internships at the University of Tokyo and IBM Research. Todd received an Early Career Research Award from the U.S. Department of Energy in 2014.

Frameworks, Programming Paradigms and Methods for Extreme Computing

Serge G. Petiton[1]
[1]*Maison de la Simulation/CNRS*
and University Lille 1, Sciences et Technologies, Lille, France

Abstract

Exascale hypercomputers are expected to have highly hierarchical architectures with nodes composed by lot-of-core processors and accelerators. The different programming levels (from clusters of multi-processors nodes loosely connected to tightly connected lot-of-core processors and/or accelerators) will generate new difficult algorithm issues. New languages and frameworks should be defined and evaluated with respect to modern state-of-the-art of scientific methods. Methods have to be redesigned and new ones introduced or rehabilitated, in particular in terms of communication optimizations and data distribution.

Since more than a decade, joint Japanese-French researches were developed on several topics associated with these challenges. In this talk, we present some of these researches. In particular, we survey the main results obtained using graph of PGAS written tasks experimented on the K AICS computer, with YML developed in France and XMP developed in Japan. We also discuss on the auto-tuning Hybrid Krylov methods developed with the University of Tokyo and the University of Tsukuba, in this framework, and present some results on large clusters.

Hence, we focus on YML with its high level language allowing to automate and delegate the managements of dependencies between loosely coupled clusters of processors to a specialized tool controlling the execution of the application using XMP written tasks. In this framework, we present some basic matrix operations utilized on Hybrid Krylov methods on clusters of accelerators. We discuss some recent experiments on a cluster of accelerators concerning comparison between orthogonal, incompletely orthogonal and non-orthogonal Krylov Basis computing. Then, we will discuss some results obtained on a cluster of accelerators to compute eigenvalues with respect to restarting strategies. We will survey some auto/smart-tunning strategies we proposed and evaluated for some of the Krylov method parameters We conclude proposing the integration of several obtained results toward intelligent numerical computing on the road to exascale computing and beyond.

Biography

Prof. Serge G. Petiton received the B.S. degree in mathematics, in 1982, the M.S. in Applied Mathematics, in 1984, the M.E. in Operating System degree, in 1985, the Ph.D. degree in computer science, in 1988, and the "Habilitation à diriger des recherches", in 1993, from Pierre and Marie Curie University, Univ. PARIS 6. He was post-doc student, registered at the graduate school, and junior researcher scientist at the YALE University, 1989-1990. He has been researcher at the "Site Experimental en Hyperparallelisme" (supported by CNRS, CEA, and French DoD) from 1991 to 1994. He also was affiliate research scientist at Yale and visiting research fellow in several US laboratories, especially in NASA-ICASE and the AHPCRC during the period 1991-1994. Since then, Serge G. Petiton is Professor at the Scientific and Technical University of Lille, Univ. Lille 1. Serge G. Petiton leads the "Methodoly and Algorithmic

Programming" group of the CNRS "Laboratoire d'Informatique Fondamentale de Lille", and he participated to the INRIA Saclay "Grand Large" project. He is lecturer in several French universities and was lecturer at the University of Tsukuba, at the Hohai University in Najing, and at A*star in Singapore. He is director of the board of the ORAP association (launched in 1994 by CNRS, INRIA and CEA) to promote HPC and he participates to several French and International HPC committees. From 2009 to 2012, he leads the HPC and GRID group at the CNRS-Japanese French laboratory on Informatics (JFLI) in Tokyo. Serge Petiton was the French P.I. ANR-JST French-Japanese project "Framework for Post-Petascale Programming and Computing" (FP3C), from 2010 to 2014, and also work with several US universities and laboratories including LBNL. Since 2012, Serge G. Petiton has a half time CNRS senior position at the "Maison de la Simulation" in Saclay where he created the "Groupe de Recherches Avances en Calculs Exascales" (GRACE).

Serge G. Petiton has been scientific director of more than 22 Ph.D.s and has authored more than 100 articles on international journals and conferences. His main current research interests are in "Parallel and Distributed Computing", "Post-Petascale Auto/smart-tuned Dense and Sparse Linear Algebra", and "Language and Programming Paradigm for Extreme Modern Scientific Computing"; targeting big data applications.

Multi-SPMD Programming Paradigm for Extreme Computing

Miwako Tsuji[1]
[1]*RIKEN AICS, Kobe, Japan*

Abstract

Supercomputers in the exa-scale era would consist of a huge number of nodes arranged in a multi-level hierarchy. There are many important challenges to exploit such systems. Through the Japanese-French FP3C (Framework and Programming for Post-Petascale Computing) project and the subsequent RIKEN/AICS-CNRS/MDLS agreement, we have been focusing on the challenges for the extreme computing such as scalability, programmability, reliability and energy efficiency, etc..... In this talk, I focus on the scalability, programmability and reliability and introduce a multi-SPMD programming environment based on workflow and PGAS (Partitioned Global Address Space) programming models for parallel programming.

Biography

Dr. Miwako Tsuji is a research scientist at RIKEN Advanced Institute for Computational Science since 2013. She is a member of the architecture development team of flagship 2020 (post K computer) project, since the project was started in 2014. Her research interests are programming model, tools and fault tolerance for large scale systems.

Dense solver for eigenvalue problems on Petascale and towards post-Peta-scale systems

Toshiyuki Imamura[1]
[1]*RIKEN Advanced Institute for Computational Science, Kobe, Japan*

Abstract

It is needless to say that high-performance numerical libraries or framework are one of the significant software building blocks for the development of large-scale scientific simulation codes. One of the missions of AICS is to strength the usability of K computer system but also towards future supercomputer systems. Our team develops a high-performance parallel eigenvalue solver for dense symmetric/Hermitian eigenvalue problems, namely EigenExa. We consider a couple of performance factors from parallel algorithm to parallel implementation. On one hand for the parallel algorithm, we take advantage of dense-band transformation, which can resolve bottleneck of the memory bandwidth. Though K computer system has relatively richer memory bandwidth, byte/flop rate is less than 0.5. This fact implies that Level 3 BLAS routines have strong advantages rather than Level 1 and 2 BLAS routines. On another hand for parallel implementation, we investigate communication avoidance technique to the most time-consuming part of eigenvalue solver. This technique reduces the communication overhead and improves system efficiency (reducing the ratio of CPU-idle time). In this talk, the outline of our mission towards post-petascale supercomputer system, and especially, the current status of our outstanding numerical library, EigenExa, will be presented.

References

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[2] T. Fukaya, and T. Imamura, Performance evaluation of the EigenExa eigensolver on Oakleaf-FX: tridiagonalization versus pentadiagonalization, in Proc. PDSEC2015.

Biography

Toshiyuki Imamura is currently a Team Leader of Large-scale Parallel Numerical Computing Technology at AICS, RIKEN. He was a researcher at CCSE JAERI (1996-2003), a visiting scientist at HLRS (2001-2002), and an associate professor at the Univ. Electro-Communications (2003-2012). Since 2012, he has been with RIKEN. His research interests include HPC, Automatic-Tuning, and eigenvalue computation. He and his colleagues are one of the finalists for Gordon Bell Prize in SC05 and SC06.

The Joint Laboratory for Extreme Scale Computing: Investigating the challenges of post petascale scientific computing

Franck Cappello[1]
[1] *Argonne National Laboratory, Argonne, IL, USA*

Abstract

Extreme scale computing is critical to fuel discovery in scientific domains with high societal impact such as climate science, material science, health science and cosmology.

At the time where extreme scale scientific simulation and data analytics are transitioning from Petascale to Exascale, it becomes more and more difficult for a single institution to develop all the R&D needed to run efficiently complex applications on these very expensive systems. Beyond 2025, the scientific community will face even bigger challenges with the end of Moores law.

The Joint-Laboratory has been established initially between Inria and UIUC in 2009 as an attempt to combine their R&D excellence to address Petascale challenges. The joint-lab successes motivated its evolution toward the JLESC that focuses on Exascale computing and beyond. In 2016, the JLESC has 6 partner institutions: UIUC/NCSA, Inria, Argonne National Laboratory, Barcelona Supercomputing Center, Jülich Supercomputing Center and Riken/AICS.

In this talk, we will present the JLESC and several of its collaborations and successes in key topics: Applications, Workflow, Performance optimization, I/O & storage, Resilience, Energy optimization, Applied Mathematics.

Biography

Franck Cappello is Senior Computer Scientist at Argonne National Laboratory.He is director of the Inria-UIUC-ANL-BSC-JSC-Riken/AICS Joint-Laboratory on Extreme Scale Computing. Before moving to ANL in 2013, he held from 2009 a joint position at Inria and University of Illinois at Urbana Champaign. From 2003 to 2008, at Inria, he initiated and directed the Grid5000 project in France, a nation wide computer science Platform for research in large scale distributed systems. He has authored papers in the domains of Fault tolerance, High Performance Computing, Desktop Grids and Grids and contributed to more than 80 Program Committees. He is editorial board member of the international Journal on Grid Computing, Journal of Grid and Utility Computing and Journal of Cluster Computing. He is a steering committee member of ACM HPDC And IEEE/ACM CCGRID. He was the Award co-chair for IEEE/ACM SC15, Program co-chair for ACM HPDC2014, Test of time award chair for IEEE/ACM SC13, Tutorial co-Chair of IEEE/ACM SC12, Technical papers co-chair at IEEE/ACM SC11, Program chair of HiPC2011, program cochair of IEEE CCGRID 2009, Program Area co-chair IEEE/ACM SC'09, General Chair of IEEE HPDC 2006.

Challenges for Parallel Programming Models and Languages of post-petascale and extreme scale computing

Mitsuhisa Sato[1]
[1]*RIKEN AICS, Kobe, Japan*

Abstract

First of all, I will present an overview of activities in AICS for JLESC (Joint Laboratory on Extreme Scale Computing). For extreme scale computing, there are many challenges and issues including architectures and programming models to exploit billions of parallelism and the limitation of power consumption. Toward a post-petascale system as the next of Japan's petascale facility, the K computer, the project, FLAGSHIP2020, has been launched to develop and deploy the post-K computer. In this talk, researches on programming languages and tools in the project will be described, and challenges for parallel programming models and languages in extreme scale computing will be addressed.

Biography

Mitsuhisa Sato received the M.S. degree and the Ph.D. degree in information science from the University of Tokyo in 1984 and 1990. He was a senior researcher at Electrotechnical Laboratory from 1991 to 1996, and a chief of Parallel and distributed system performance laboratory in Real World Computing Partnership, Japan, from 1996 to 2001. From 2001, he was a professor of Graduate School of Systems and Information Engineering, University of Tsukuba. He has been working as a director of Center for computational sciences, University of Tsukuba from 2007 to 2013. Since October 2010, he is appointed to the research team leader of programming environment research team in Advanced Institute of Computational Science (AICS), RIKEN. Since 2014, he is working as a team leader of architecture development team in FLAGSHIP 2020 project in RIKEN AICS.

Talk Session
(Day 2)

Tuesday, February 23

Necessity and feasibility of brain-scale simulations at cellular and synaptic resolution

Markus Diesmann[1,2]
[1]*INM, Jülich Research Centre, Jülich, Germany*
[2]*RWTH Aachen University, Aachen, Germany*

Abstract

The cortical microcircuit, the network comprising a square millimeter of brain tissue, has been the subject of intense experimental and theoretical research. The talk first introduces a full-scale model of the microcircuit at cellular and synaptic resolution [1] comprising about 100,000 neurons and one billion local synapses connecting them. The emerging network activity exhibits fundamental properties of in vivo activity. Despite this success, the explanatory power of local models is limited as half of the synapses of each excitatory nerve cell have non-local origins. The second part of the talk therefore argues for the need of brain-scale models [2] to arrive at self-consistent descriptions and addresses the arising technological and theoretical questions: Are simulations of the required size feasible [3][4][5] and are full-scale simulations required as opposed to downscaled representatives [5]? The study presents data for the K and JUQUEEN computers providing an outlook for exascale systems.

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Biography

Prof. Markus Diesmann is Director of Institute of Neuroscience and Medicine (INM-6), Computational and Systems Neuroscience, Director of Institute for Advanced Simulation (IAS-6), Theoretical Neuroscience, Research Center Jülich, Germany, and full professor (W3) in Computational Neuroscience at Faculty of Medicine, RWTH University Aachen, Germany.

He studied Physics and Computer Science at Ruhr University with a year of Cognitive Science at University of Sussex, UK. He carried out PhD studies at Weizmann Institute of Science, Israel, and Albert-Ludwigs-University. In 2002 he received his Ph.D. degree with distinction from Faculty of Physics, Ruhr-University Bochum, Germany. From 1999 Prof. Markus Diesmann worked as Senior Staff at Dept. of Nonlinear Dynamics, Max-Planck-Institute for Dynamics and Self-Organization, Goettingen, Germany. He was an Assistant Professor of Computational Neurophysics at Albert-Ludwigs-University, Freiburg, Germany before gaining experience as a Unit Leader and Team Leader at RIKEN Brain Science Institute, Wako City, Japan. His main scientific interests include correlation structure of neuronal networks, models of cortical networks, simulation technology and supercomputing.

Scalasca and VI-HPS for K computer

Brian Wylie[1]
[1] *Jülich Supercomputing Centre, Forschungszentrum Jülich, Jülich, Germany*

Abstract

The open-source Scalasca toolset [www.scalasca.org] for scalable performance analysis of large-scale parallel applications has supported profiling and tracing of MPI, OpenMP and hybrid MPI+OpenMP on K computer since early in 2013. Scalasca2, based on the community-developed Score-P instrumentation and measurement infrastructure and SIONlib library for scalable task-local file I/O, included support for K computer in August 2014. These tools have been used to analyse the execution efficiency of scientific applications on K computer with up to 82,944 MPI processes and 663,552 OpenMP threads, and investigate remediation of critical performance and scalability issues.

Hands-on training in the use of these and other tools that assist parallel application developers to diagnose programming errors and optimise performance is provided via the Virtual Institute – High Productivity Supercomputing [www.vi-hps.org] by JSC and eleven partner institutions. RIKEN AICS hosted a VI-HPS Tuning Workshop in March 2014 using K computer, and a follow-up will take place 24-26 February 2016.

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Biography

Brian Wylie is a research scientist at Jülich Supercomputing Centre of Forschungszentrum Jülich since 2004, where he is a developer of the Scalasca toolset for scalable performance analysis of large-scale parallel applications. Additional responsibilities include application engagement and coordinating training activities of the Virtual Institute – High Productivity Supercomputing encompassing the series of VI-HPS Tuning Workshops, bespoke courses and tutorials featuring hands-on use of VI-HPS parallel program developer tools held on four continents.

Upgrading Climate Models for Diverging Architectures

Naoya Maruyama[1]
[1]*RIKEN Advanced Institute for Computational Science, Kobe, Japan*

Abstract

Architectural diversity, as exemplified by the current and upcoming computing systems, presents pressing challenges to high performance computing applications. Global climate modeling, for instance, is confronted with the necessity of adopting new architectures to further expand the capability of simulation models. While model implementations have been typically designed and optimized for a class of machine architecture at hand, such software designs lead to poor portability in both functionality and performance in the presence of architectural divergence. To address this problem, our joint project, originally started within AICS but now expanded with atmospheric computing experts in Germany, France, and Japan, explores feasibilities and effectiveness of modern programming methodologies such as high-level domain specific languages. This talk presents our past achievements and discusses future plans.

Biography

Naoya Maruyama is a Team Leader at RIKEN AICS, where he leads the HPC Programming Framework Research Team. His team focuses on high-level parallel frameworks for computational science applications to support productive and highly efficient computing with large-scale parallel systems such as RIKEN's K computer. He is also the Principal Investigator for a JST Post Petascale System Software Project, where his team has been developing domain-specific programming models for mesh-based and particle-based applications that are primarily targeted to achieve high scalability and efficiency on large-scale GPU machines. He won several awards, including a Gordon Bell Prize in 2011. He received Ph.D. in Computer Science from Tokyo Institute of Technology in 2008.

ALCF Operations Best Practices and Highlights

Mark Fahey[1]
[1] *Argonne National Laboratory, Argonne, IL, USA*

Abstract

The Argonne Leadership Computing Facility currently operates the 5th fastest computer in the world – an IBM Blue Gene/Q named Mira. Mira has 786,432 Power PC cores in 32 cabinets while only using roughly 2.5 MW of power (lowest by far of the top 5.) We will describe the ALCF and its computing resources and then highlight some of the best practices for operations. We will also look to the future describing coming computational resources and some of the challenges and opportunities that are coming.

Biography

Mark Fahey has over 20 years of experience working with high performance computers. As Director of Operations, he is responsible for all day-to-day operations for the 48 rack Blue-Gene/Q Mira supercomputer and assures the machine meets extremely high measured standards for availability and reliability. Previously, Dr. Fahey served as the Deputy Director at the National Institute for Computational Science within the University of Tennessee Knoxville. He has also served as the Scientific Computing Group Leader at NICS where his group, comprised of PhD level application scientists. Dr. Fahey was also Senior Research Staff in the Scientific Computing Group within the National Center for Computational Sciences at Oak Ridge National Laboratory. He developed XALT and ALTD library tracking infrastructures in use at various HPC centers around the world, and has written over 50 papers in the area of high performance and scientific computing. Mr. Fahey received his B.A. from St. Norbert College in 1992 and his Ph.D. from the University of Kentucky in 1999.

Operation of the K computer and the facilities

F. Shoji[1], K. Yamamoto[1], A. Uno[1], A. Kuroda[1], K. Minami[1], T. Tsukamoto[1]
[1] *Operations and Computer Technologies Division, RIKEN AICS, Kobe, Japan*

Abstract

The K computer is well known as one of the fastest supercomputer in the world. K computer has completed in June 2012 and public use has started since September 2012 and operation of the K computer is highly stable so far. For example, Cumulative number of users is more than 1,500 and submitted jobs are more than 1,000,000. The ratio of irregular system down time is no more than 2.3%.

In this presentation, we report recent operation status of the K computer and we analyze trends of faults and failures. In order to reduce energy costs, analysis of power consumption is very important. Here we introduce our approaches for reduction of energy consumption and how can we apply them to the operation improvements.

References

[1] Mitsuo Yokokawa et al., The K computer: Japanese next-generation supercomputer development project, Proceedings of the 17th IEEE/ACM International Symposium on Low-power Electronics and Design, ISLPED'11, pages 371–372, 2011.

[2] Keiji Yamamoto et al., The K computer Operations: Experiences and Statistics, Procedia Computer Science, Volume 29, 2014, Pages 576–585.

Biography

- 2005–2012 Research & Development Scientist/Team leader, Next-generation Supercomputer development Center, RIKEN
- 2010– Team head/Division director, Advanced Institute for Computational Science, RIKEN
- Research interests: Operation and the improvement of massively parallel systems

The POP project

Jesus Labarta[1]
[1] *Barcelona Supercomputing Center, Barcelona, Spain*

Abstract

The POP project is a recently started EU Center of Excellence with the long term objective of improving the practices and widen the reach of performance analysis in parallel programming. The increasing complexity of our systems makes extremely important to increase the amount of insight on the actual behavior of applications and systems to be able to gain such insigth in the minimum possible time. This information is needed to improve the efficiency of operation of our infrastructures and to maximize the productivity of our code refactoring efforts.

At the short term, the project focuses on providing performance assessment services. Target "customers" for these services include application developers and infrastructure operators, but also vendors and users.

The talk will present the project, some of the technologies and methodology being used. We envisage that this type of activities and coordination efforts shuld be enlarged by setting up cooperations at a borader internationa level.

Biography

Jesus Labarta is full professor on Computer Architecture at the Technical University of Catalonia (UPC) since 1990. Since 1981 he has been lecturing on computer architecture, operating systems, computer networks and performance evaluation. His research interest has been centered on parallel computing, covering areas from multiprocessor architecture, memory hierarchy, programming models, parallelizing compilers, operating systems, parallelization of numerical kernels, performance analysis and prediction tools.

Since 2005 he is responsible of the Computer Science Research Department within the Barcelona Supercomputing Center (BSC). He has been involved in research cooperation with many leading companies on HPC related topics. His major directions of current work relate to performance analysis tools, programming models and resource management. His team distributes the Open Source BSC tools (Paraver and Dimemas) and performs research on increasing the intelligence embedded in the performance analysis tools. He is involved in the development of the OmpSs programming model and its different implementations for SMP, GPUs and cluster platforms. He has been involved in Exascale activities such as IESP and EESI where he has been responsible of the Runtime and Programming model sections of the respective Roadmaps. He leads the programming models and resource management activities in the HPC subproject of the Human Brain Project.

Global Optimization Study of metal oxide nanocluster and Their Application in Catalysis

Ramesh Ch. Deka[1], Pakiza Begum[1], Snigdha Dutta[1], Plaban J. Sarma[1], S. M. Woodley[2], C. R. A. Catlow[2]
[1]*Department of Chemical Sciences, Tezpur University, Napaam, Tezpur 784 028, Assam, India*
[1]*Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, United Kingdom*

Abstract

Stable and metastable structures of metal oxide nano structures such as $(NiO)_n$, $(SnO2)_n$, $(CeO2)_n$ are generated for n = 1 to 32 using Monte Carlo global optimization techniques implemented in a newly developed program called KLMC[1]. The genetic algorithm was used in global optimization. Pre-screening of structures involves relaxation to minimization with a cheaper energy function - based on interatomic potentials. About 50 different nanoclusters were generated for the larger cluster size. For each of the cluster size, three most stable structures were reoptimized at all-electron DFT level. The most stable structure of $(NiO)_{30}$ is shown in Figure 1.

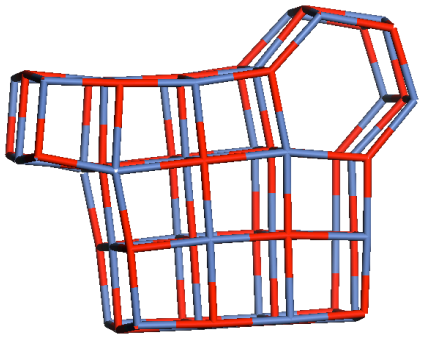

Figure 1: Most stable structure of $(NiO)_{30}$ cluster

The HOMO-LUMO energies, magnetic properties and catalytic properties[2] of the clusters are calculated.

References

[1] Woodley, S. M. Knowledge Led Master Code, http://www.ucl.ac.uk/klmc/Software (accessed 2012).

[2] Deka, P, Deka, R. C. and Bharali, P. New J. Chem. 38 (2014) 1789-1793.

Biography

Prof. Ramesh Ch. Deka, Department of Chemical Sciences, Tezpur University
Academic Records:
- M. Sc. 1994, Gauhati University, Assam

- Ph. D. 1998, National Chemical Laboratory, Pune

Awards and Honors:

1. Alexander von Humboldt Fellowship, 2003
2. Hidustan Platinum Award by the Catalysis Society of India, 2005
3. Professor H. C. Goswami award by Assam Science Society, 2013
4. Bronze Medal, Chemical Research Society of India 2013
5. UKIERI (UK India Education and Research Initiative) Fellowship 2013
6. DST-JSPS Special Lecture Tour Award 2015

Research Interests:

- Theoretical Chemistry, Molecular Modelling, Drug Design and Catalysis

Publication:

- Over 140 research papers in international journals

Development of Library for Future Meteorological Simulations: SCALE

Hirofumi TOMITA[1], Team SCALE[1],
[1]*RIKEN Advanced Institute for Computational Science, s-nishizawa@riken.jp*
7-1-26 Minatojima-minami-machi Chuo-ku, Kobe, Hyogo 650-0047, Japan

Abstract

In the climate/meteorological model, most of processes, especially physical processes, are based on empirical rules and hypotheses. This leads to large uncertainties in simulation result from the deficiency of model. To evaluate the reliability of the simulations, direct comparison between various schemes is necessary through conducting the sensitivity of schemes. So far, many inter-model comparison studies have obtained a lot of fruitful knowledge. However, it is difficult to clarify what is an origin that bears the difference of results, because there are many differences in the components and schemes between the models. For this purpose, we have developed a library and environment for climate/meteorological simulations, SCALE (Scalable Computing for Advanced Library and Environment; Nishizawa et al 2015, Sato et al 2015), which is freely available on the web site (http://scale.aics.riken.jp/) on the BSD2 license. We intend to a direction to easily compare between the physics/dynamics schemes.

To use future HPCs efficiently, collaborating with computer scientists is a crucial issue. We have started it with computer science teams in AICS. The higher-resolution simulation still requires appropriate choice or modification of the schemes. In my talk, I also briefly talk about a possibility of international collaboration for climate modeling.

References

[1] Nishizawa et al. 2015: Influence of grid aspect ratio on planetary boundary layer turbulence in large-eddy simulations, Geosci. Model Dev., 8, 3393–3419.

[2] Sato et al. 2015: Impacts of cloud microphysics on trade wind cumulus: which cloud microphysics processes contribute to the diversity in a large eddy simulation? PEPS, 2:23.

Biography

Hirofumi TOMITA (Dr.Eng.)
Curriculum Vitae:
- Apr. 1988 – Mar. 1994: Department of aeronautics and astronautics, The University of Tokyo
- Apr. 1994 – Mar. 1996: Master course of aeronautics and astronautics, Graduate school of engineering, The University of Tokyo
- Apr. 1996 – Mar. 1999: Doctor course of aeronautics and astronautics, Graduate school of engineering, The University of Tokyo
- Apr. 1999 – Mar. 2002: Post Doctor Researcher, Frontier Research System for Global Change
- Apr. 2002 – Mar. 2007: Researcher, Frontier Research Center for Global Change
- Apr. 2007 – Mar. 2009: Senior Scientist, Frontier Research Center for Global Change
- Apr. 2009 – Dec. 2010: Senior Scientist, Research Institute of Global Change, JAMSTEC
- Jan. 2011 – present: Team Leader, RIKEN/Advanced Institute for Computational Science, Computational Climate Science Research Team

- Apr. 2014 - present: FLAGSHIP 2020 Project Deputy Project Leader / Team Leader, Application Development Team

Award:

- The 2011th JMSJ paper award from the Meteorological Society of JapanNiwa, Y., H. Tomita, M. Satoh, and R. Imasu (2011): A Three-Dimensional Icosahedral Grid Advection Scheme Preserving Monotonicity and Consistency with Continuity for Atmospheric Tracer Transport, J. Meteor. Soc.Japan, Vol. 89, 255–268

- Masaki Satoh and Hirofumi TOMITA, The 2006th gakkai-award from the Meteorological Society of Japan,
"Development of global cloud resolving model using a quisi-homogenious grid and simulation of cloud clusters in the tropics by the model"

- Hirofumi TOMITA, The 2005th ryumon-award from Japan Society of Fluid Mechanics,"Development of Nonhydrostatic Atmospheric General Circulation Model using an Icosahedral Grid"

Frameworks for Large-scale parallel simulations

Jun Makino[1]
[1]*AICS, Kobe, Japan*

Abstract

In this talk, I present two complementary efforts our group in AICS and Leiden University are pursuing. One is to develop frameworks which support the development of new parallel applications with specific techniques, such as the particle method and the finite difference method. The other is to develop a framework on which existing parallel applications can be integrated to provide multi-physics and/or multi-scale capabilities. As examples of the first approach, I discuss FDPS and Formura developed in AICS. As an example of the latter, I discuss AMUSE developed in Leiden.

Biography

Jun Makino received Phd from the University of Tokyo. After his PhD, he worked University of Tokyo, the National Astronomical Observatory of Japan, and Tokyo Institute of Technology. Since Apr 2014, he is a subleader of the exascale computing project and the team leader of the Co-design team, AICS, RIKEN. His research interests are stellar dynamics, large-scale scientific simulation and high-performance computing.

HIVE - Parallel remote visualization system, its concept and functions

Kenji Ono[1]
[1] *Advanced visualization research team, RIKEN AICS, Kobe, Japan*

Abstract

Our team is currently developing HIVE visualization system for large-scale datasets which are generated from massively parallel computing environments. The developed HIVE system has features of scalability, flexibility, multi-platform, and extensibility. The key technology that forms the backbone of HIVE is adopting the combination of commodity APIs, i.e. GLES (OpenGL for Embedded Systems) and GLSL (OpenGL Shading Language), to construct highly scalable sort-last type parallel rendering sub-system. Since these APIs supply compact instruction set, it is easy to learn to describe new shader algorithms and effects. We built parallel ray-tracing core with GLES/GLSL APIs. Another important technology is the image compositing algorithm that scales on massively parallel environments. We have developed novel flexible and scalable compositing algorithm for arbitrary number of processors. We had already achieved to generate an 8k image using 82,944 processors on the K-computer, and we are now tackling to visualize various computed results on the K-computer and to try to add new functionality, e.g., visual-analytic approach. Both the parallel coordinate and the fiber surface methods are combined with HIVE. Visual analytic framework allows us to explore data space with interactivity, which will give us new insight or clue for scientific discovery.

Biography

Kenji Ono is currently a team leader of Advanced Visualization research team at AICS, RIKEN. He received his degrees of Dr. Eng. in mechanical engineering from Kumamoto university, Japan in 2000. From 1990 to 2001, he was a research engineer in Nissan Motor company and, from 2001 to 2004, he was an associate professor at the University of Tokyo. His research fields are Computational Fluid Dynamics, parallel high-performance computing and visualization for large-scale dataset.

Computational Simulations for Advanced Manufacturing and Energy Storage

Srdjan Simunovic[1]
[1] *Oak Ridge National Laboratory, Oak Ridge, USA*

Abstract

Additive Manufacturing (AM), also known as 3D printing, is a manufacturing technology for producing parts by selectively melting and solidifying feedstock material in powder, wire or sheet form. The functional performance of the AM-manufactured parts is strongly influenced by the material microstructure, residual stresses, and distortion that build up during the manufacturing process. Understanding the underlying physical phenomena, and formulating this knowledge into predictive computational models, are crucial for the AM technology development. Another focus subject of our research is modeling of advanced storage systems. Both problems contain multi-physics and multi-scale phenomena that require development of new mathematical, computational and experimental approaches. We will review the current research and methods for modeling the AM processes and energy storage devices from micro to macro scale, and describe the experimental programs for model validation. The role of High Performance Computing (HPC) on modeling and coupling of different length scales and physics phenomena will be discussed. We will describe future directions for research and development in the two fields, and discuss collaboration opportunities in modeling, computing, and experimentation.

References

[1] Talagani, M.; et al.; SAMPE Journal, 51(4), 2015.

[2] Allu, S.; et al.; J Power Sources, 246, pp 876-86, 2014.

[3] Stershic, A. J.; Simunovic, S.; Nanda, J.; J Power Sources, 297, 2015.

[4] Pannala, S.; et al.; J Applied Physics, 118(7), 072017, 2015.

[5] Computational Engineering and Energy Sciences; http://energy.ornl.gov

[6] Oak Ridge Leadership Computing Facility; https://www.olcf.ornl.gov

Biography

Srdjan Simunovic is a Distinguished Research Staff in the Computer Science and Mathematics Division, Oak Ridge National Laboratory, USA and Joint Faculty at the University of Tennessee, Knoxville, the University of Tennessee, Chattanooga, and Purdue University . He holds MSc and PhD degrees in computational mechanics from Carnegie Mellon University in Pittsburgh, USA, and BSc from University of Split, Croatia. His research expertise includes computational modeling of materials and structures, composite materials manufacturing, battery modeling, process modeling of additive manufacturing, and development of multi-physics codes for high performance computing.

Poster Session

Monday, February 22

17:00-18:00

P-01

Ensemble Data Assimilation of GSMaP precipitation into the nonhydrostatic global atmospheric model NICAM

Shunji Kotsuki[1]
[1]*Data Assimilation Research Team, RIKEN Advanced Institute for Computational Science*

Abstract

It is generally difficult to assimilate precipitation data into numerical models mainly because of non-Gaussianity of precipitation variables and nonlinear precipitation processes. Lien et al. (2013, 2015) proposed to use an ensemble Kalman filter approach to avoid explicit linearization of models, and a Gaussian transformation (GT) method to deal with the non-Gaussianity of precipitation variables. Lien et al. pioneered to show that using an EnKF and GT helps improve the forecasts by assimilating global precipitation data both in a simulated study using the SPEEDY model, and in a real-world study using the NCEP GFS and TRMM Multi-satellite Precipitation Analysis (TMPA) data.

This study extends the previous study by Lien et al. and assimilates the JAXAs Global Satellite Mapping of Precipitation (GSMaP) data into the Nonhydrostatic Icosahedral Atmospheric Model (NICAM) at 112-km horizontal resolution. This study newly develops a method to construct the two GTs (forward and inverse GTs) for observed and forecasted precipitation using the previous 30-day precipitation data. Using this new forward GT, precipitation variables are transformed to be the Gaussian variables, and we succeeded in improving the forecasts by assimilating the GSMaP precipitation. We also found the use of the inverse GT, so that we can obtain observation-like precipitation fields transformed by observation-based inverse GT from the model forecasts. Moreover, we also explore online estimation of model parameters related to precipitation processes using precipitation data. This presentation will include the most recent progress up to the time of the symposium.

P-02

File System Performance on The K computer

Keiji Yamamoto[1], Atsuya Uno, Fumiyoshi Shoji
[1]*RIKEN Advanced Institute for Computational Science*

Abstract

The K computer has two types of file system. One is global file system (GFS), the other is local file system (LFS). GFS is used from login node and the capacity is 30PB. LFS is used from compute node and the capacity is 11PB. LFS is composed of 2,592 OSSes (Object Storage Server) and 5,184 OSTs (Object Storage Target). In this poster, we describe configuration and performance of the local file system.

P-03

Processing of XFEL still images with a reference oscillation data set for crystal structural analyses of cytochrome c oxidase

Fangjia Luo[1], Atsuhiro Shimada[1], Kunio Hirata[2], Tomitake Tsukihara[1], Shiya Yoshikawa[1]

[1]*Picobiology Institute, Graduate School of Life Science, University of Hyogo*

[2]*RIKEN SPring-8 Center*

Abstract

X-ray free electron laser is powerful tool which is given really high hope for generating high-resolution X-ray crystallography data developed recently. But with the enormous energy the laser has, the crystal or data can be easily disrupted. That requires us to update the data collecting method. Two methods for XFEL data collection are currently underdeveloping. The serial femtosecond crystallography (SFX) requires many crystals subjected to the subsequent X-ray pulse. The other is serial femtosecond rotation crystallography (SF-ROX). In this method a crystal mounted on a goniometer-head is exposed by the X-ray pulse and translates for the next exposure to obtain serial diffraction images with an equal rotation interval.But from diffraction images, the data quality indicator Rmerge is 24.3% which is twice of the convention value.

To obtain high quality data set from SF-ROX diffraction images we have initiated development of data processing procedure. . Our ideas are as follows: (1) A reference intensity data set is obtained by the oscillation method using crystals grown in the same batch as those used in SF-ROX method (2) Fix cell constant to those of SF-ROX data before processing. (3) Crystal orientation parameters are refined to reduce the difference between I of the reference data and I/P of the target crystal, where P stands for partiality reflection. P is a function of the distance of a reciprocal lattice point from the reflection sphere. Once orientation parameters converge well in the refinement procedure, P is estimated and the observed intensity is evaluated by the formula, I/P. The new program suite PRIME developed by Stanford, it revealed a process loop using reference obtained the origin still image data to estimated the correct intensity. But the cell constant and orientation parameter obtained from convention oscillation x-ray experiment may be more close to the correct parameter than those obtained from initial data set. Hopefully using two reference data set can help us to estimate full intensity more accuracy.

P-04

Data assimilation experiments with MODIS LAI observations and the dynamic global vegetation model SEIB-DGVM

Hazuki Arakida[1], Takemasa Miyoshi[1], Takeshi Ise[2], Shin-ichiro Shima[3], Shunji Kotsuki[1]

[1] *RIKEN Advanced Insititute for Computational Science*

[2] *Field Science Education and Research Center, Kyoto University*

[3] *Graduate School of Simulation Studies, University of Hyogo*

Abstract

We developed an ensemble data assimilation system with a dynamical global vegetation model known as the SEIB-DGVM (Spatially Explicit Individual Base Dynamic Global Vegetation Model). The model is an individual-based model, and it includes non-Gaussian and non-linear processes. In addition, the phase space changes due to the occasional establishment and death of the plants. Therefore, we used one of the particle filter methods, the Sampling Importance Resampling (SIR), which can handle these difficulties. The experiment was performed at the Larch forest of Eastern Siberia, and the state variables and parameters of the deciduous needle leaved tree and grass were estimated.

First, an Observing System Simulation Experiment (OSSE) was performed. We simulated LAI observations from the nature run with the true phenological parameters: maximum photosynthesis rate and dormancy date. By assimilating the simulated LAI observations, the parameters and other dynamical variables such as Gross Primary Product (GPP), Ecosystem Respiration (RE), and Net Ecosystem CO2 Exchange (NEE) were estimated successfully. Next, we assimilated the real-world MODIS LAI data. The results showed generally good match with the FLUXNET field observation data for NEE.

P-05

Data-centric GPU-based Adaptive Mesh Refinement

Mohamed Wahib[1]
[1]*HPC Programming Framework Research Team,*
RIKEN Advanced Institute for Computational Science

Abstract

It has been demonstrated that explicit stencil computations of high- resolution scheme can highly benefit from GPUs. This includes Adaptive Mesh Refinement (AMR), which is a model for adapting the resolution of a stencil grid locally. Unlike uniform grid stencils, however, adapting the grid is typically done on the CPU side. This requires transferring the stencil data arrays to/from CPU every time the grid is adapted. We propose a data-centric approach to GPU-based AMR. That is, porting all the mesh adaptation operations touching the data arrays to the GPU. This would allow the stencil data arrays to reside on the GPU memory for the entirety of the simulation. Thus, the GPU code would specialize on the data residing on its memory while the CPU specializes on the AMR metadata residing on CPU memory. We compare the performance of the proposed method to a basic GPU implementation and an optimized GPU implementation that overlaps communication and computation. The performance of two GPU-based AMR applications is enhanced by 2.21x, and 2.83x compared to the basic implementation.

P-06

XcalableACC: A Parallel Programming Language for Accelerated Clusters

Masahiro Nakao[1]
[1]*RIKEN Advanced Institute for Computational Science*

Abstract

The poster introduces the XcalableACC programming language for accelerated cluster systems. XcalableACC is a hybrid model of the XcalableMP directive-based language for cluster systems and the OpenACC directive-based language for accelerators. XcalableACC provides directives to define distributed array on accelerator memories and parallelize for-loop statement by using accelerators. Moreover, XcalableACC also provides directives to transfer data among accelerators directly. We have been developing an Omni XcalableACC compiler as a reference implementation.

In the poster, we will showcase the design of the XcalableACC and the implementation of the Omni XcalableACC compiler. Moreover, we will evaluate its performance and productivity through some benchmarks.

P-07

Global precipitation nowcasting by spatiotemporal extrapolation with data assimilation

Shigenori Otsuka[1]
[1]*RIKEN Advanced Institute for Computational Science*

Abstract

Spatiotemporal extrapolation is a widely-used technique for precipitation nowcasting. Motions of precipitation systems are estimated using two or more consecutive observations of precipitation patterns by radars or satellites, and the precipitation patterns are extrapolated in time and space to obtain their future patterns. We have implemented a prototype extrapolation system for the JAXAs Global Satellite Mapping of Precipitation (GSMaP) Near Real Time (NRT) product. Motion vectors based on satellite images have large uncertainties, and applying data assimilation will help improve the spatiotemporal structures of the motion vectors. The extrapolation system is implemented using the local ensemble transform Kalman filter, and tested using the real-case GSMaP global precipitation patterns.

P-08

Accelerating a non-hydrostatic ocean model with multigrid Poisson/Helmholtz solver using a GPU

Takateru Yamagishi[1]
[1]*Kobe Center, Research Organization for Information Science and Technology*

Abstract

Oceanic numerical simulations play important roles in climate studies and development of oceanic resources. Ocean circulation consists of various scale dynamics such as turbulent mixing induced by tides, descending gravity currents and their entrainment, deep convection and huge stream. Long execution is required to predict and study climate change. To resolve small processes in a huge domain with fast speed is crucial and essential to study large scale oceanic circulation. GPU is expected to meet the recent demand because of its low cost and high performance. However, few studies have been conducted on the role of GPU in ocean models and the experimental research available is insufficient to support the study of oceanic processes.

This study aims to examine the execution of a non-hydrostatic ocean model on a GPU and to create an experimental model to study small oceanic processes. We implemented a numerical, non-hydrostatic ocean model called kinaco on a GPU following basic but essential methods. We improved the models Poisson/Helmholtz (P/H) solver by optimizing the memory access, using instruction-parallelism, and applying a mixed precision calculation to the preconditioning of the P/H solver.

On the GPU (NVIDIA Tesla K20c), we achieved an execution time 4.7 times faster compared to the CPU (Fujitsu SPARC 64VIIIfx), and the GPU-implemented P/H solver became 1.5 times faster with the measures to improve the P/H solver. With the improved P/H solver, the output errors were negligible and should not significantly influence oceanic studies. This study demonstrates that a numerical ocean model is suitable for GPU implementation in terms of both high performance and output accuracy.

There is potential for further improvement in this ocean model. We have not utilized shared memory to remove redundant access to global memory, except in the parallel sum reduction kernel. We could take advantage of the specific characteristics of the numerical ocean model, such as the uniformity of some coefficients in the model equations, and the memory access could be optimized. This study shows that the application of mixed precision is an effective method and suggests that further research is needed to identify other applicable kernels and to verify them from both computational and geophysical viewpoints.

P-09

Multi-scale localization compared with 10240-member ensemble Kalman filter using real observations

Keiichi Kondo[1]
[1]*Data Assimilation Research Team, RIKEN Advanced Institute for Computational Science*

Abstract

Covariance localization plays an essential role in the ensemble Kalman filter (EnKF) with a limited ensemble size. Localization limits the influence of observations and reduces the impact of sampling errors. To treat the sampling errors, we implemented a 10240-member EnKF without localization and investigated analysis accuracy and the error covariance structures using an intermediate AGCM known as the SPEEDY model. The results showed that the analysis was much improved by assimilating distant observations. Alternatively, we also proposed and investigated a multi-scale localization method named the dual localization method which coupled two separate localization scales. The results showed consistent improvement over a traditional single localization approach. In this study, we further extend the previous studies to use the real-world observations with the non-hydrostatic icosahedoral atmospheric model (NICAM) and to investigate how well the dual localization method captures the multi-scale covariance structures and approximates the 10240-member EnKF. Performing 10240-member EnKF with realistic settings, we faced much computational challenges. This presentation includes the most recent results of the 10240-member EnKF and the comparison with dual-localization EnKF, as well as the computational aspects of the large-ensemble EnKF computations.

P-10

Eigenspectrum calculation of the O(a)-improved Wilson-Dirac operator in lattice QCD using the Sakurai-Sugiura method

Hiroya Suno[1,2]
[1]*RIKEN Advanced Institute for Computational Science*
[2]*RIKEN Nishina Center for Accelerator-Based Science*

Abstract

We have developed a computer code to find eigenvalues and eigenvectors of non-Hermitian sparse matrices arising in lattice quantum chromodynamics (lattice QCD). The Sakurai-Sugiura (SS) method is employed here, which is based on a contour integral, allowing us to obtain desired eigenvalues located inside a given contour of the complex plane. We apply the method here to calculating several low-lying eigenvalues of the non-Hermitian $O(a)$-improved Wilson-Dirac operator. Evaluation of the low-lying eigenvalues is crucial since they determine the sign of its determinant $detD$, important quantity in lattice QCD. We are particularly interested in such cases as finding the lowest eigenvalues to be equal or close to zero in the complex plane. Our implementation is tested for the Wilson-Dirac operator in free case, for which the eigenvalues are analytically known. We also carry out several numerical experiments using different sets of gauge field configurations obtained in quenched approximation as well as in full QCD simulation almost at the physical point. Various lattice sizes $L_xL_yL_zL_t$ are considered from $8^3times16$ to 96^4, amounting to the matrix order $12L_xL_yL_zL_t$ from 98,304 to 1,019,215,872.

P-11

Analysis Example of the Correlation between Application Performance and Power Consumption on the K computer

Akiyoshi Kuroda[1], Yoshito Kitazawa, Kiyoshi Kumahata,
Toshiyuki Tsukamoto, Kentaro Koyama, Hikaru Inoue, Kazuo Minami
[1]*RIKEN Advanced Institute for Computational Science*

Abstract

In high-performance computing, an increase of power consumption along with the advancement of system performance becomes a major concern. We had expected that there were no applications but the LINPACK benchmark program which used almost all parts of the K computer and exceeded power consumption limits. However, we found the cases that power consumption of some applications exceeded such limits by huge-size job executions occupying the entire system of the K computer due to advances of massively parallel coding. In this study, we evaluated power consumption by associating the characteristics of application performance, such as the efficiencies of floating-point calculation performance, main memory throughput, L2 cache throughput, L1 data cache throughput, and integer calculation performance. From these evaluations, we found that main memory throughput had greater influence on power consumption than floating-point calculations. We will also introduce some of the analysis example.

P-12

Assimilating Himawari-8 Brightness Temperature: A Case Study on Typhoon Soudelor (2015)

Takumi Honda[1]
[1]*Data Assimilation Research Team, RIKEN Advanced Institute for Computational Science*

Abstract

The Japan Meteorological Agency started full operations of the new geostationary meteorological satellite Himawari-8 in July 2015. Himawari-8 is the first of a series of the third-generation geostationary meteorological satellites including NOAAś GOES-R (planned for launch in 2016), producing about 50 times more data with more channels and 3 times more observing frequency than the previous generation. In August 2015, Himawari-8 successfully captured rapid intensification of Typhoon Soudelor (2015), the strongest northwestern Pacific typhoon in the summer of 2015 with minimum central pressure of 900 hPa. In this study, we assimilate brightness temperature from Himawari-8 using our new ensemble data assimilation system called SCALE-LETKF and investigate its impact on the analyses and forecasts of Soudelor.

P-13

Universal quantum criticality in two-dimensional interacting Dirac electrons

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Abstract

We investigate the metal-insulator transition of two-dimensional interacting electrons with massless Dirac-like dispersion, describe by the Hubbard models on two geometrically different lattices: honeycomb and π-flux square lattices. By performing large-scale quantum Monte Carlo simulations followed by careful finite-size scaling analyses, we find that the transition from semi-metallic to antiferromagnetic insulating phases is continuous and evaluate the critical exponents with a high degree of accuracy for the corresponding universality class, which is described in the continuous limit by the Gross-Neveu model. We furthermore discuss the fate of the quasiparticle weight and the Fermi velocity across this transition.

P-14

A near-real-time weather analysis and forecast system based on the SCALE-LETKF

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Abstract

Numerical weather prediction (NWP) is a unique area of computational science, making accurate prediction of the future state of the environment in the real time, and the prediction can also be soon verified. It is achieved by running an NWP model, acquiring weather observations, and assimilating the observational data to find the best-estimate initial conditions. Following the typical NWP procedure used in operational weather prediction centers over the world, we built an experimental near-real-time weather analysis and forecast system based on the SCALE-LETKF, utilizing the Scalable Computing for Advanced Library and Environment (SCALE)-LES model and the Local Ensemble Transform Kalman Filter (LETKF) data assimilation method. Using the K computer, the system has been routinely running for 8 months since 7 May, 2015. A large amount of the analysis and forecast data has been collected. These data are important for verifying the performance and stability of the SCALE-LETKF, which benefits the development of both the numerical model and the data assimilation system.

P-15

Addressing Fault Tolerance on Extreme Scale Systems

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Abstract

Applications typically mitigate faults on high performance computing systems by employing checkpoint/restart, whereby applications periodically save their state to checkpoint files and can later restart from those files if a failure occurs. While this technique is straightforward, it can incur high overhead for large-scale jobs. The Scalable Checkpoint/Restart Library (SCR) was designed to reduce this overhead by using in-system storage to cache checkpoint files. In this poster, we will give an overview of SCR and highlight research efforts that aim to further reduce the overhead of checkpointing.

P-16

Spack: A Tool for Managing Exascale Software

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Abstract

The complexity of HPC software is quickly outpacing existing software management tools. HPC applications and tools alike depend on bleeding edge compilers, numerical libraries, runtime systems, and messaging libraries, and the software ecosystem is expected to become even more diverse at exascale. Performance experts and researchers frequently need to experiment with many different builds of the same code in order to get the best performance, but building large software stacks is often a daunting and time consuming task.

In this poster, we describe Spack (https://github.com/LLNL/spack), a tool used to build, test, and share production applications and tools at LLNL, NERSC, ANL, ORNL, and other HPC sites. Spack provides a novel, recursive specification syntax that allows parametric builds of packages and their dependency DAGs. It allows arbitrary library and runtime combinations to coexist in the same environment, and its combinatorial versioning system allows developers to experiment with many different variants of a software stack to do performance parameter studies.

P-17

Study on 2015 typhoon Nangka with the SCALE-LETKF system

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Abstract

The typhoon Nangka (Typhoon No.11 in 2015) brought in a heavy rainfall event in the Kobe city. It caused the disruption to train services. In this study, we carried out retrospective data assimilation and forecast experiments with the SCALE-LETKF system which couples a highly parallelized large eddy simulation weather model (SCALE-LES) with an ensemble data assimilation method, the local ensemble transform Kalman filter (LETKF). First, the sensitivity of the horizontal and vertical localization scales to the typhoon Nangka case was investigated. Second, the predictability of the Kobe rainfall event was also investigated with ensemble forecasts. The results of the sensitivity experiments show that changing localization scales have little impacts on the results of intensity and track forecast. In addition, that of forecast experiments show that the Kobe rainfall event prediction is very difficult, but the reproducibility of the Kobe rainfall event is able to increase with a high-resolution experiment.

P-18

Performance evaluation of the tall-skinny QR factorization on recent parallel systems

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[3]*JST CREST*
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Abstract

Computing the QR factorization of a tall and skinny matrix is one of important building blocks in numerical computations. One of its famous applications is orthogonalization of vectors, which is, for example, required in projection methods for solving linear systems and eigenvalue problems. The Gram-Schmidt and Householder QR algorithms are well-known, and the TSQR and Cholesky QR (and its variants) algorithms now attract the interest of researchers from the viewpoint of high performance computing. Each of these algorithms has different characteristics in terms of computation cost, communication coast in parallel computing, and numerical stability. There are many studies in which the runtime of these algorithms on parallel systems are theoretically compared, however experimental evaluation is also important. This is because theoretical studies often assume simple machine models, which does not necessarily reflect actual situations.

In this poster, we present the results of experimentally comparing these algorithms by using recent parallel systems including the K computer. We measure the runtime with changing the size of matrix and the number of processes. We show the breakdown of the runtime, which would help one discuss the performance on upcoming systems whose hardware specifications (e.g. flops, bandwidth, latency, etc.) will be different from those of current systems. We also give some results on numerical stability, which is also vital in applications. We expect these results would contribute to both further development of these algorithms and appropriate selection of these algorithms in each application program.

P-19

An evaluation and improvement for HPCG on the K computer

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Abstract

The LINPACK benchmark has been used as a metric of supercomputer performance. Recently, there are opinions that the LINPACK benchmark is biased toward computational performance, ignoring other important performance aspects such as data transfer speed. These data transfer speed is important for modern supercomputers and applications in today. As a result, the LINPACK benchmark is considered as an unrealistic metric. Thus, the high performance conjugate gradient benchmark (HPCG) has been proposed to establish an alternative metric that better reflects the performance of realistic applications in modern supercomputers. This benchmarks the speed for solving symmetric sparse linear system equations using the conjugate gradient method preconditioned by the multi-grid symmetric Gauss-Seidel smoother. HPCG has features (1) a coefficient matrix is derived from an unstructured grid used in finite element type methods. Memory access is indirect. Therefore, unlike LINPACK, its performance strongly depends on memory access. (2) Preconditioned conjugate gradient (PCG) methods are widely used in many scientific and engineering fields.

We have evaluated and attempted to improve the performance of HPCG on the K computer using an early version obtained prior to its official announcement. In the performance evaluation on the K computer, it was found that the parallel scalability was extremely good by weak-scaling measurement, the single CPU performance was totally low, and almost all running time depended on two dominant kernels. Therefore, it was focused to improve the single CPU of these two dominant kernels in our improving efforts describing below.

First, memory arrangement was made continuous. In the original code, matrix rows are allocated separately. Thus rows are located discontinuously in memory space. This discontinuous should disturb efficient cache-memory utilization. Second, the routine for the symmetric Gauss-Seidel, it is used for smoothing and relaxation in a multi-grid preconditioner, was modified into be multi-thread parallelize. The original code runs this kernel in sequential not in parallel, due to data dependencies in the algorithm of the Gauss-Seidel method. In this tuning, special technique was employed. Third, the loop structures of the kernels were optimized for the K computer CPU using some optimization techniques. And finally we improved miscellaneous parts of the benchmark in the K, such as the running parameter and the routine for matrix data optimization.

As a result, running time of HPCG was improved 19 times faster. And the K computer remarked 0.461 PFLOPS using 82,944 nodes. This score ranked 2nd in the world at SC15.

P-20

Overview of the HPCI Shared Storage

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Abstract

The HPCI Shared Storage is the data sharing infrastructure of HPCI, total 22.5PB single view Gfarm file system is open for all HPCI users. Gfarm file system is a network file system that supports scalable I/O performance in widely distributed geographically environment.

HPCI Shared Storage data servers are located at AICS, TokyoTech, and The University of Tokyo. And the master meta data servers are located at the University of Tokyo, slave servers are located at the University of Tokyo and AICS. The meta data transactions are transferred from the master server to slave servers.

HPCI shared storage is available from all the HPCI super computer resources via SINET4/ SINET5 network. HPCI Shared Storage supports HPCI single sign-on authentication (GSI-auth), if a user wants to transfer computational results to the HPCI shared storage after the computational session, the user does not have to login again to the HPCI shared storage. HPCI Shared Storage also supports automatic file replication, adopts 2 file replicas in default for data protection.

In April of 2015, we found 150000 data corrupted files in TokyoTech data servers. Even though most of files rescued by replica files, total 923 files are lost in this failure. As the result of the analysis, this is the typical silent data corruption. To cope with the silent data corruption, the periodical data integrity check using file digest feature in Gfarm is introduced in HPCI Shared Storage. This periodical data integrity check enables data corrupted file detection within one week. In addition to the periodical data integrity check, we also introduced the operation guideline based on ITIL.

Considering of the past 3 years operation, we HPCI Shared Storage team is designing the next-generation HPCI Shared Storage System.

P-21

An investigation of impacts of surface observations on a sudden severe rainstorm forecast

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Abstract

To investigate a pinpoint forecast of a sudden severe rainstorm event occurred on September 11, 2014 around Kobe city, this study performs a series of data assimilation (DA) experiment using Local Ensemble Transform Kalman Filter (LETKF) with the JMA-NHM (NHM-LETKF). In this event, a cumulonimbus generated suddenly near the central Kobe city around 0800 JST. It developed rapidly within 10-minutes, and brought heavy rainfall over 50 mm h-1 from 0830 JST to 0930 JST.

As the first investigation of the LETKF experiment, the control run was performed only assimilated radar reflectivity and radius wind data of Phased Array Weather Radar (PAWR) which located in Osaka University. We originally installed surface observational instruments named POTEKA II at 8-locations in Kobe city, and get surface data every 30-seconds. We also performed other DA experiments assimilated with both PAWR data, and temperature and relative humidity data of POTEKA II. Since we have already known that POTEKA II data has an observational bias, two DA experiments with the raw POTEKA II data (NOBC) and the bias corrected POTEKA II data (BC) were performed. Horizontal resolution of NHM-LETKF is 1-km and ensemble size is 100. In CTRL, LETKF was cycled every 30-seconds from 0745 JST to 0830 JST. In NOBC and BC, the initial time was set to 0700 JST for spin up run. In addition, forecast experiments initialized at 0830 JST were performed to investigate the impacts of surface DA on forecasts.

After 50-cycle of LETKF, intensive echoes over 35 dBZ appeared at 2-km elevation in CTRL. Surface rainfall was also expressed in the forecast experiment, but the intensity is smaller than that of a conventional observation by JMA. In NOBC, surface relative humidity decreased because of an observational bias, and resulted in a negative effect for developing a cumulonimbus. On the other hand, the rainfall intensity obviously improved in a forecast experiment of BC. At a LETKF step, 16 POTEKA II data were available, only 0.01 % of PAWR data. However, surface DA has a potentiality to contribute an improvement of the forecast accuracy in a sudden severe rainstorm event.

P-22

Proposal for Dynamic Task Parallelism in PGAS Language XcalableMP

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Abstract

In the field of high performance computing, large-scale clusters based on many core processor such as Intel Xeon Phi have been deploying in many cites according to Top500 Lists. In order to get a good performance on these clusters, we have to consider a high level of parallelization on the node as well as overlap of computations and communication between the nodes due to using a lot of cores efficiently. Therefore, we focus on the task parallelism, which facilitates the parallelization where work is generated dynamically, and reduces the cost of synchronization using task-to-task synchronization by the dependency description on each thread rather than the barrier of all cores.

On the other hands, Message Passing Interface (MPI) is used widely for programming distributed memory systems. However, its low productivity is an important problem because it forces programmer to describe the data distribution explicitly and primitive API for inter-node communication. To solve these problems, the partitioned global address space (PGAS) parallel programming model has emerged as a usable distributed memory programming model. XcalableMP (XMP) is a PGAS parallel programming language that extends base languages such as C and Fortran with directives in OpenMP-like style. XMP enables the parallelization of serial source code with additional directives to describe the data distribution, synchronization, and the consistency among them over multiple nodes with distributed memory systems.

For the above reasons, we propose the tasklet directive in PGAS language XMP to describe easily for dynamic task parallelism on distributed memory systems, and implement it to Omni XcalableMP Compiler that is a source-to-source translator to change from XMP directive to MPI code. The tasklet directive is now under consideration by XMP Specification Working Group for next version of XMP. Therefore, this research is one of a proposal function. In this poster, we evaluate the performance and productivity of block cholesky factorization with the tasklet directive to compare it with StarPU that is a task programming library on distributed memory systems developed at INRIA. As a result, the performances of block cholesky factorization with tasklet directive are same or a little higher than that of StarPU version in most cases. In addition, we obtained the high productivity because the amount of code is smaller with XMP version than the StarPU version, and XMP version is the almost same as the data dependency of single node version with OpenMP in spite of the distributed memory systems.

P-23

A skew-tuned shuffling for MapReduce on large scale supercomputers

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Abstract

MapReduce processing system treats the data as a Key-Value(KV) object and distributes KV in each compute-node before the reduce processing phase. If KVs are evenly distributed among nodes, then we can improve the reduce processing time. However, existing distribution algorithms scalability are not good because of the centralized approach. We are studying a new scalable algorithm to equalize the number of KVs processed by each node. In this study, we confirmed that the reduce processing time is shortened, but total time of MapReduce processing is increased from the evaluation of PageRank calculation.

P-24

High-resolution global atmospheric data assimilation experiments with an ensemble Kalman filter

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Abstract

It is crucial to develop a numerical weather prediction system including data assimilation in order to predict the extreme weather such as heavy rainfalls and typhoons in the post-K era. We have been developing the NICAM-LETKF system to assimilate the conventional observations, satellite microwave radiances from AMSU-A (Advanced Microwave Sounding Unit-A), and satellite-based global precipitation data GSMaP (Global Satellite Mapping of Precipitation). The NICAM-LETKF may be run at very high resolution, or may provide boundary conditions for even higher resolution systems. Improving the NICAM-LETKF performance is at the center of enhancing mesoscale predictability for better preparedness for severe weather events well in advance.

Data assimilation experiments have been conducted with NICAM-LETKF at 112- and 28-km horizontal resolution with 100 ensemble members. Higher resolution experiment can reproduce the precipitation field well by assimilating precipitation observations. We need to keep improving the physical and computational performances of NICAM-LETKF to increase the resolution and the ensemble size, and to assimilate "Big Data" from the next-generation observations.

P-25

Program Development Tools for the Exascale Area

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Abstract

On our way to exascale systems, both applications and architectures are becoming increasingly complex and so are their interactions. This drives the need for practical, easy-to-use, and comprehensive program development tools that continue to provide basic functionality at the largest scales as well as address the new challenges imposed, e.g., by novel architectures, memory systems, or the use of accelerators.

This poster will highlight several ongoing projects at Lawrence Livermore National Laboratory (LLNL) in this area, describe their basic features, their availability and future plans: from production performance tools, such as Open—SpeedShop or mpiP that provide an easy-to-generate overview of basic performance metrics, to MemAxes and Ravel, two next generation tools for memory allocation and message traffic analysis; from the widely used STAT debugging tool, designed to detect hangs at large scale quickly, to novel race checkers and MPI correctness tools. Complemented is this wide range of tools with Caliper, a simple annotation API that application developers or runtimes can use to expose additional context to tools. Examples for the latter are program phases, data structure information, or dependencies in task based systems. This information is combined with measured too data to enrich the semantic information and aid in precise attribution of performance and debugging data to code elements.

Combined, these tools provide both debugging and performance information to a deliver both correct and efficient applications at scale and are therefore an important part of the exascale software stack. More information on each tool is available on the URLs listed or via https://scalability.llnl.gov/.

P-26

Introduction of Research Activities for GPU Computing at Large-scale Parallel Numerical Computing Technology Research Team on AICS

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Abstract

Utilizing many-core accelerators such as GPUs is an important research topic for large-scale numerical computing. In this poster, we introduce recent research activities on GPU computing at our team, Large-scale Parallel Numerical Computing Technology Research Team on AICS. This poster mainly includes the following two topics:

(1) High performance level-2 BLAS kernels: We are developing some linear algebra kernels such as Basic Linear Algebra Subprograms (BLAS) using CUDA for NVIDIA GPUs. We have proposed sophisticated implementations of level-2 BLAS routines: GEMV (general matrix-vector multiplication) [1] and SYMV (symmetric matrix-vector multiplication) [2]. Depending on usage conditions such as the problem size and the kind of GPU, our implementations vary some parameters including the thread-block size automatically. As a result, they achieved higher throughput and performance stability with respect to the matrix size on multiple GPU architectures when compared to the existing implementations such as CUBLAS. We have also developed the routines for multi-GPU environments. This poster includes the performance evaluation results on up to 4 GPUs.

(2) Short length floating-point formats (SLFP) [3] (work-in-progress): Although the required precision depends on the purpose of the computation, most numerical libraries only support IEEE's 32- and 64-bit floating point formats. In order to tune the performance of numerical software in terms of precision, we are trying to introduce new floating point formats that have shorter bit-length than the IEEE standard's. By eliminating waste data movement in the computation using the shorter length formats, we expect to improve the computation speed and its energy efficiency. In this poster, we show our proposal method and the preliminary evaluation results on a GPU.

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P-27

Development of In-Situ Visualization tool VISMO

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Abstract

We have been developing an In-Situ Visualization tool named VISMO [1]. It is mainly for PIC (Particle-In-Cell) simulations and has basic visualization methods for particles, scalar and vector data. We have already united the tool and a PIC simulation code [2], and executed the linked code on the Plasma Simulator supercomputer (Hitachi SR16000 Model M1, POWER7) using 2,048 CPU cores in 2013. The code could output the images successfully.

One of the most serious problems about In-Situ visualization is its interactivity. In In-Situ visualization, not raw data but images are saved. It means that researchers cannot change the viewing point or visualization methods after their simulations end. We have recently incorporated a function into VISMO and developed a special viewer. The function saves visualized objects, namely isosurfaces, slices, arrows and streamlines, as point clouds. The special viewer reads the point clouds and displays them. The objects are observed from all the viewing points interactively. The sizes of point clouds are controlled by users.

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P-28

Tapas: a programming framework for hierarchical particle algorithms

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Abstract

We propose Tapas, a programming framework for hierarchical particle method designed to be highly productive, high performance, and practical. The framework allows programmers to write applications in an implicitly parallel, straight forward recursive notation. It is implemented in standard C++11 language and exploits meta-programming techniques to automate intra-process and inter-process parallelism including LET construction, and GPU execution. We port ExaFMM, a highly tuned implementation of the Fast Multipole Method, on Tapas and evaluate performance on TSUBAME2.5 supercomputing platform.

P-29

Particle Based Volume Rendering on Vector Machines

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Abstract

The data produced by computer simulations are too large to analyze them by the traditional interactive visualization on PCs recently. In-situ visualization is considered to be a solution to this problem. In this method, a simulation code is united with a visualization code, and the united code executed on a supercomputer visualizes the data and saves images on the storages instead of saving raw result data simply. To realize in-situ visualization of unstructured data on vector machines, we have vectorized particle based volume rendering method and examined its performance on Earth Simulator.

P-30

Implementation of an FEM application using coarray

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Abstract

Coarray is a part of specifications of the Fortran 2008. In Fortran 2008 specification, it has feasibility of an implicit one-sided communications in the user programs. This poster shows that coarray representations are implemented as an alternative to MPI non-blocking communications kernel in FFB, which is an application of the finite element method that solves the unsteady incompressible Navier-Stokes equations. The FFB is a subset of FIBER provided by RIKEN AICS. The goal of this research is both to discover the method of coarray implementations and to evaluate of the effectiveness of coarray in FEM program. In original FFB, the communication kernel carries out exchange the data between the neighboring nodes by using non-blocking MPI communications. These communications need indirect array address references in order to get the base address and communication size of arrays. In pure MPI implementation, the sender knows only the receive partner and the size, receiver knows only the transmission partner and the size. But in the coarray implementation, the origin process needs all communication partner and size in advance. Therefore we implement to gather the array index information as coarray in order to get the data from other nodes when we use coarray. As the result, the coarray program, which is compiled by the Omni XMP compiler, achieved the equivalent of performance of the pure MPI program on an SMP machine. Now we are trying to achieve to carry out the coarray implementation on a distributed memory machines.

P-31

Sequential data assimilation for single-molecule FRET photon-counting data

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Abstract

Data assimilation is a statistical method designed to improve the quality of numerical simulations in combination with real observations. We have developed a sequential data assimilation method that incorporates one-dimensional time-series data of single-molecule FRET (smFRET) photon-counting into conformational ensembles of biomolecules derived from replicated molecular dynamics (MD) simulations. A particle filter using a large number of replicated MD simulations with a likelihood function for smFRET photon-counting data is employed to screen the conformational ensembles that match the experimental data. In the poster, we show the details of our method as well as preliminary results obtained by an application to the smFRET data of protein folding dynamics.

P-32

Molecular crowding effect on GTP hydrolysis reaction in Ras-GAP complex

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Abstract

Macromolecular crowding effects have essential role in biomolecular system. Such effects have been extensively investigated experimentally, and also in classical Molecular Dynamics (MD) calculations. However, in the quantum chemistry level, those effects are not investigated due to the computational costs and methodological difficulties. In this study, we studied the molecular crowding effect on the GTP hydrolysis reaction in Ras-GAP complex by QM/MM RWFE method, which can take crowding effects into account with a reasonable computational cost. We modeled a crowding environment by adding 7 BSAs to the system as a crowder, and refined the reactant and transition states of the hydrolysis reaction.

The structural difference around GTP were not significant between solution and crowding environment. However, there is a large difference in the electrostatic potential imposed by the surroundings. We will also discuss about fluctuations of electrostatic potential and protein structure in the presentation.

P-33

Development of 3D reconstruction program for coherent diffraction patterns obtained by XFEL

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Abstract

3D structural analysis for single particles using X-ray free electron laser (XFEL) is a new structural biology technique. This technique enables us to observe the molecules, which are hard crystallized such as biological molecules and living tissue, in the state close to nature. Using a large number of 2D diffraction patterns obtained by XFEL from different orientations relative to the molecule, a 3D structure of the molecule in Fourier space (structure factor) can be reconstructed. Through inverse Fourier transformation of the structure factor, 3D structure of the molecule in real space can be restored. However, it is extremely difficult to control the orientation of the single particle to the beam incidence direction. In addition, the phase information, which is required for inverse Fourier transform, is lost in the observed diffraction patterns. In order 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 (cryo-EM) data. Cryo-EM provides 2D real space images, which can be assembled to build a 3D structure. Some of the methods using real space image for 3D reconstruction can also be applied to Fourier space. Preliminary results using simulated diffraction patterns will be presented.

P-34

An Optimized FPGA-based Accelerator for Big Scale Deep Neural Network

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Abstract

Deep Neural Network (DNN), a human brain inspired machine learning algorithm, has recently been shown to provide much better performance than other machine learning algorithm. It has been applied to fields like computer vision, speech recognition, nature language process and bioinformatics where it has been shown to produce state-of-art results on various tasks.However, a conventional general CPU or GPU cannot meet the performance requirement when the data is huge and DNN scale is big.

In this work, we proposed a mapping algorithm to map the neurons to on-chip networks by using computing the minimum hops. This mapping algorithm is applied to three cases: (1)all the neurons of the whole deep neural network can be mapped to single acceleration node; (2)all the neurons of single layer can be mapped to single acceleration node; (3) only part of neurons in a single layer can be mapped to single acceleration node. This mapping algorithm can effectively reduce the latency and improve the network throughput. Thereby, the performance is improved.

P-35

A hybrid approach to extract structural information from small number of 2D X-ray coherent diffraction patterns

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Abstract

Recently, X-ray free electron laser (XFEL) emerged and started to be used as fourth-generation X-ray sources that provide a femto-second X-ray pulse with the peak brilliance of at least one billion times higher than the one employed at synchrotrons. These new X-ray sources offer possibilities of providing new biological structural information.

We present a new hybrid approach for structural modeling using XFEL diffractions from non-crystalline biomolecular sample. Reconstruction of a 3D structure requires a large number of diffraction patterns; however, in the current XFEL experiments with biological systems, the analysis often relies on a small number of 2D X-ray coherent diffraction patterns. In this sturdy, we are exploring new algorithms to identify plausible 3D structural model from limited experimental data. Computational algorithms are used to generate hypothetical structural models that are in agreement with the experimental data. We established a protocol to assess the agreement between the candidate model structures and the target XFEL diffraction pattern and showed that XFEL data can be used to study the conformational transitions of biological molecules. And also, we have estimated the XFEL beam intensity strength that is required to detect conformational differences observed in the biological systems with different sizes, such as a protein molecule and ribosome complex.

The proposed algorithm can be combined with molecular mechanics approaches, such as molecular dynamics simulations and normal mode analysis, to generate a large number of candidate model structures to perform hybrid structural modeling.

P-36

Development of multi-resolution simulation methods for model of reaction with large conformational changes in biological system

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RIKEN Advanced Insititute for Computational Science

Abstract

Proteins exhibit conformational fluctuations around a native structure or transitions between multiple conformers to function under physiological conditions. Molecular dynamics (MD) simulation of protein has been widely used to investigate conformational dynamics, stability and structure-function relationships. We have developed novel high-performance MD software, GENESIS, to perform the simulations efficiently on K computer and PC clusters. Large conformational changes in response to reaction in biological system, however, are still difficult to be simulated using all atom force fields due to the slow time-scale and large space-range of motions. To overcome the difficulty, we have also developed new structure-based coarse-grained (CG) models describing domain motions and conformational changes between states. We discuss novel conformational sampling algorithms by using the CG models in biomolecular simulations.

P-37

Development of a direct numerical simulation model for water-droplet laden flow

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Abstract

We developed a direct numerical simulation model to examine interaction between air and water droplet. The model consists of air part that is governed by Navier-Stokes equation without explict assumption on viscosity term and the first law of thermodynamics, and water part in which motion and change in radius of water droplets are considered. The change in droplet radius in the model is due to phase change and collision/coalescence.

After finishing the mathematical formulation of the model, we have tested the performance on various computers including laptop and K computer. The results of test cases, e.g., gravitational fall of water droplet or rate of change in radius under constant supersaturated environment, are reasonable compared with laboratory experiments and analytical solutions.

It is indicated that the developed model can be potentially utilized for simulations of more realistic conditions and will provide useful data for future studies that aim to examine air-water interactions such as meteorological researches.

P-38

Application of a Meteorological Large Eddy Simulation Model to Practical Atmospheric Phenomena

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Abstract

A basic library for weather and climate simulations, named SCALE (Scalable Computing for Advanced Library and Environment), has been developed by Team SCALE at RIKEN AICS for a future high-resolution atmospheric simulation on an LES scale (Nishizawa et al., 2015; Sato et al., 2015). SCALE has been producing several leading results for cloud dynamics by ideal LES experiments with super-high resolution (e.g. Sato et al. 2015, PEPS; Sato et al. 2014, 2015, SOLA). We are now trying to apply a real atmospheric simulation by this model.

The time-slice experiments of five days including one-day spin-up period were conducted from May 31 to September 30 in 2008 and 2010. The boundary condition was given by the output of the operational Global Spectral Model (GSM). The horizontal spatial resolution is 7.5km and 2.5km for outer and inner domains, respectively. The precipitation was estimated by the cloud microphysics scheme (Tomita, 2008, JMSJ) for both domains. The peaks of observed rainfall distribution, located in the southern areas of Japan and the central mountain areas, were well reproduced by SCALE. On the other hand, the simulated precipitation intensity depends on the parameters in the microphysics scheme. The additional sensitivity experiments were conducted to improve the representation of precipitation intensity. From the results of that, it was shown that the parameters related to the terminal velocity of rain have the largest impact on the precipitation intensity. Finally, we quantitatively evaluated the performance of SCALE under the real atmospheric condition in summer of 2008, 2010, and 2011 as well as the present climate (SPA_m01) of MRI-AGCM3.2S.

P-39

CONeP: A Cost-effective Online Nesting Procedure for Regional Atmospheric Models

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Abstract

We propose the Cost-effective Online Nesting Procedure (CONeP) for regional atmospheric models to improve computational efficiency. The domain nesting method is used to express both the large-scale environment and fine structures simultaneously. This method is adopted in many regional atmospheric models, including the Weather Research and Forecasting Model (WRF) Advanced Research WRF (WRF-ARW; Skamarock et al. 2008) model. The simple implementation of the domain nesting method is an offline nesting. Because the simulations for the outer and inner domains are carried out individually, the history data of the outer domain simulation should be saved in files. As a result, data storage needs become quite large to satisfy an appropriate time interval for the data transfer. To resolve this problem, Michalakes (1997) implemented online nesting by way of a straightforward extension from offline nesting.

In the online nesting, data is transported from outer domain to inner domain through the inter-node communication. In this conventional procedure (CNV), computations are executed sequentially for each domain. In CNV, users cannot freely determine the number of computational nodes, considering computational efficiency. In CONeP, the processes are split into multiple subgroups, and each subgroup manages a different domain. The computations for each domain are executed in parallel. Because users can assign an appropriate node number to each domain, the model with CONeP is computationally efficient.

We implemented the CONeP on the SCALE-LES model (Sato et al. 2015; Nishizawa et al. 2015), which is a regional atmospheric model developed by RIKEN AICS. To demonstrate the superiority of CONeP over the CNV, we measured the elapsed time on the K computer. We conducted two cases of experimental settings, which are triple-nested domain setting and quad-nested domain setting. The elapsed time with CONeP is remarkably shorter than that with CNV using the same number of computational nodes. Comparing results of the quad-nested domain setting with that of the triple-nested domain setting, the advantage of CONeP becomes more significant as the number of nesting domains increases.

Considering the future architecture of supercomputer, strong scaling will become more difficult on the future HPC than current. Thus, the framework of CONeP is necessary to adjust process numbers to the problem size of each domain. In this sense, we can say that CONeP is a promising nesting procedure, directed toward the future of HPC.

P-40

Preliminary Implementation of Omni OpenACC Compiler for PEZY-SC Processor

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Abstract

Recently, accelerators are widely used for improving performance per watt. At Green 500, which is ranking of energy-efficient supercomputer, the top ten systems are equipped with accelerators in November 2015. The top system is Shoubu Supercomputer at RIKEN, which is developed by ExaScaler in Japan. The accelerator of the system is PEZY-SC processor, which has 1024 cores. ExaScaler provides PZCL as programming environment for PEZY-SC. PZCL is based on OpenCL however kernel description is different from OpenCL. PEZY-SC programming in PZCL is complex and programmers need to write many codes for data and computation offloading. In recent years, OpenACC gathers attention for accelerator programming. OpenACC is a directive-based programming interface for accelerators, which allows the programmer to express the offloading of data and computations to accelerators to simplify the porting process for legacy CPU-based applications. Some commercial and research compilers support OpenACC and most of them generate CUDA or OpenCL code for GPUs. Thus, there was no compiler supporting PEZY-SC because PZCL is not completely same with OpenCL. It is expected that OpenACC brings good productivity for PEZY-SC. Therefore we have implemented an OpenACC compiler for PEZY-SC, using Omni OpenACC compiler originally targeted to NVIDIA GPU. We evaluated the compiler by using N-body simulation in single and double precision. The performance of the OpenACC/PEZY-SC version is comparable to the PZCL/PEZY-SC version. When using single precision, the performance of the OpenACC/PEZY-SC version is reasonable compared with OpenACC/K20X, while when using double precision, it is about a twentieth part of the OpenACC/K20X because reciprocal square root is implemented by software. From the viewpoint of productivity, OpenACC version is very simple code by using directives compared with PZCL version. The SLOC (Source Lines Of Code) of OpenACC version is fewer than that of the PZCL version, so it has high productivity. Our future works are implementing the compiler features such as reduction, and optimization by compiler or extended directives.

P-41

Coarse-graining approaches for elucidating crowding effects in cells

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Abstract

The macromolecular crowding alters the thermodynamics and kinetics of biological reactions and processes in living cells. Here, to broaden our view of in vivo crowding effects, we have evaluated the stabilization on macromolecular association due to volume exclusion of crowding by using both simulations and a theory with a coarse-grained model of a bacterial cytoplasm. Degrees of stabilization evaluated by the simulations and theory were in good agreement each other. For ordinary proteins, the stabilization in the modeled cytoplasmic space was less than ?3 kBT. The present study using the simple model would provide some controls for further studies on in vivo crowding.

P-42

Parallel Implementation of molecular dynamics by combining multiple program/multiple data with multiple time step integrator

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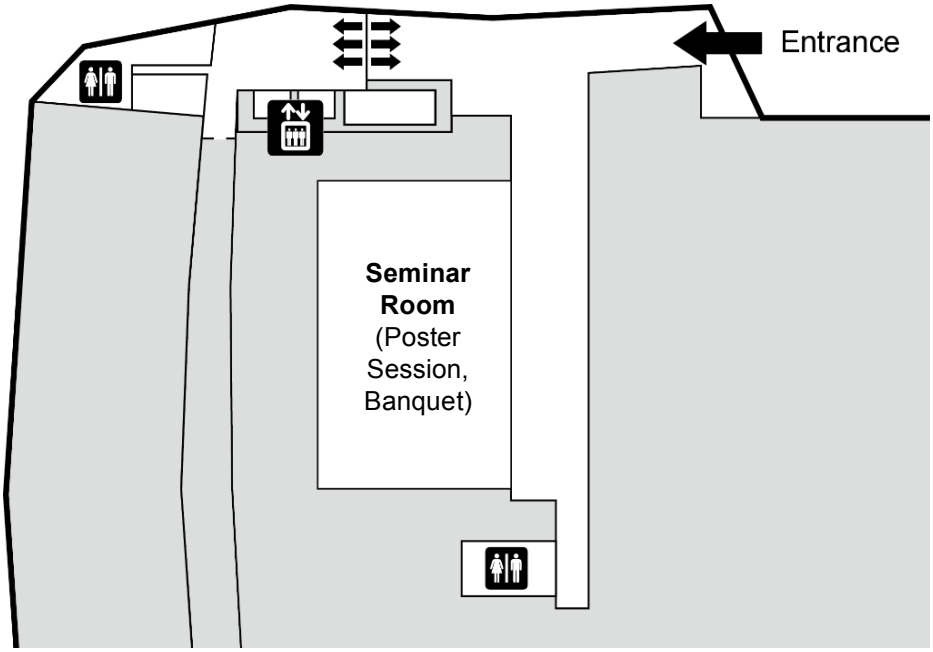
Abstract

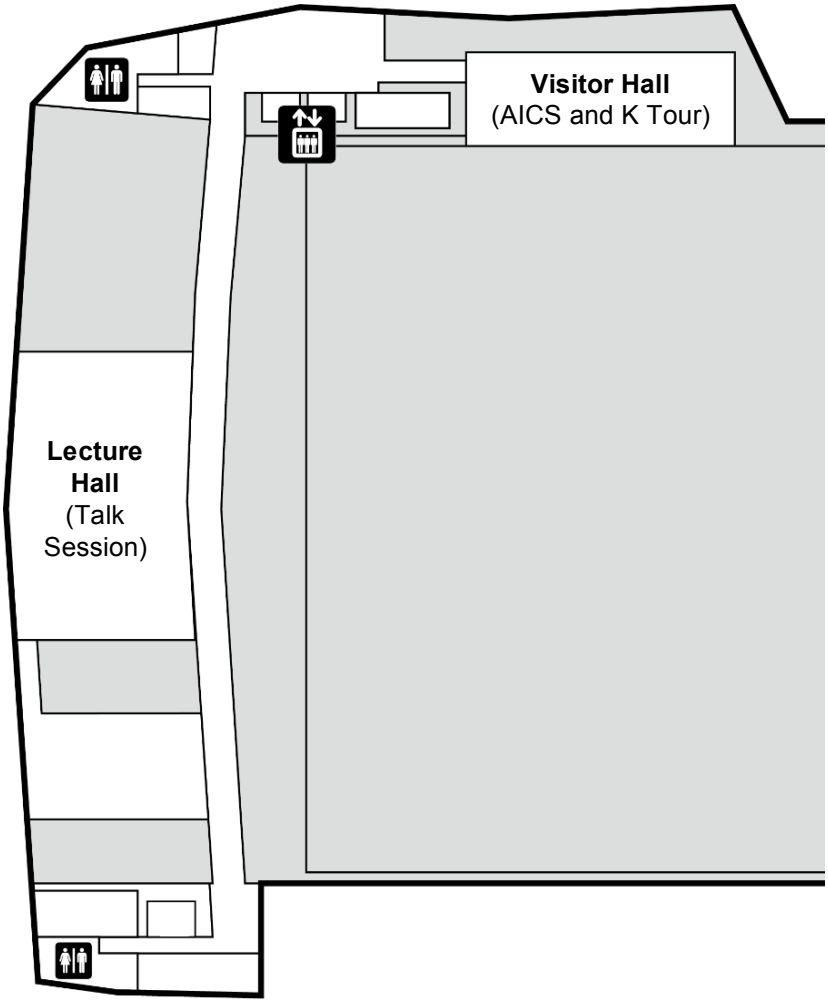
Molecular dynamics (MD) simulation is a very useful tool to understand various chemical and biological systems in atomic detail, but has a problem in computational time due to a large gap between long simulation time and small integration time step. For a small system, long time MD could be available by making use of specially designed supercomputers for MD or general purpose Graphics Processing Unit (GPU). For large scale MD on massively parallel supercomputers, increasing available number of processors from efficient parallelization is very important. Here we present efficient parallelization schemes to increase the available number of processors for MD of large systems using massively parallel supercomputers. First, we make use of a multiple-program, multiple-data approach by separating computational resources responsible for real space and reciprocal space interactions. Second, we assign the same domain decompositions between real and reciprocal spaces. Third, we assign integrations in both spaces. Fourth, the computer nodes assigned for reciprocal space interactions are also involved in real space interactions when reciprocal space interactions are not necessary in the multiple time step integrator. Our new implementation was tested on the K computer. Despite K does not include graphic processing unit (GPU) inside, and we make use of double precision floating points for all computations, we could obtain a very good performance result for big systems consisting of 1 million, 8.5 million, and 28 million atoms systems just increasing the parallel efficiencies. One MD cycle with the PME calculations for systems containing 1 million, 8.5 million, and 28 million atoms could be finished within 2.8 ms, 5.4 ms, and 8 ms without any multiple time step integrators. With multiple time step integrators, one cycle MD integration could be finished within 2.4 ms, 3.4 ms, and 7 ms, corresponding to 72 ns/day, 50 ns/day, and 24 ns/day MD simulations assuming 2fs time step.

Floor Map

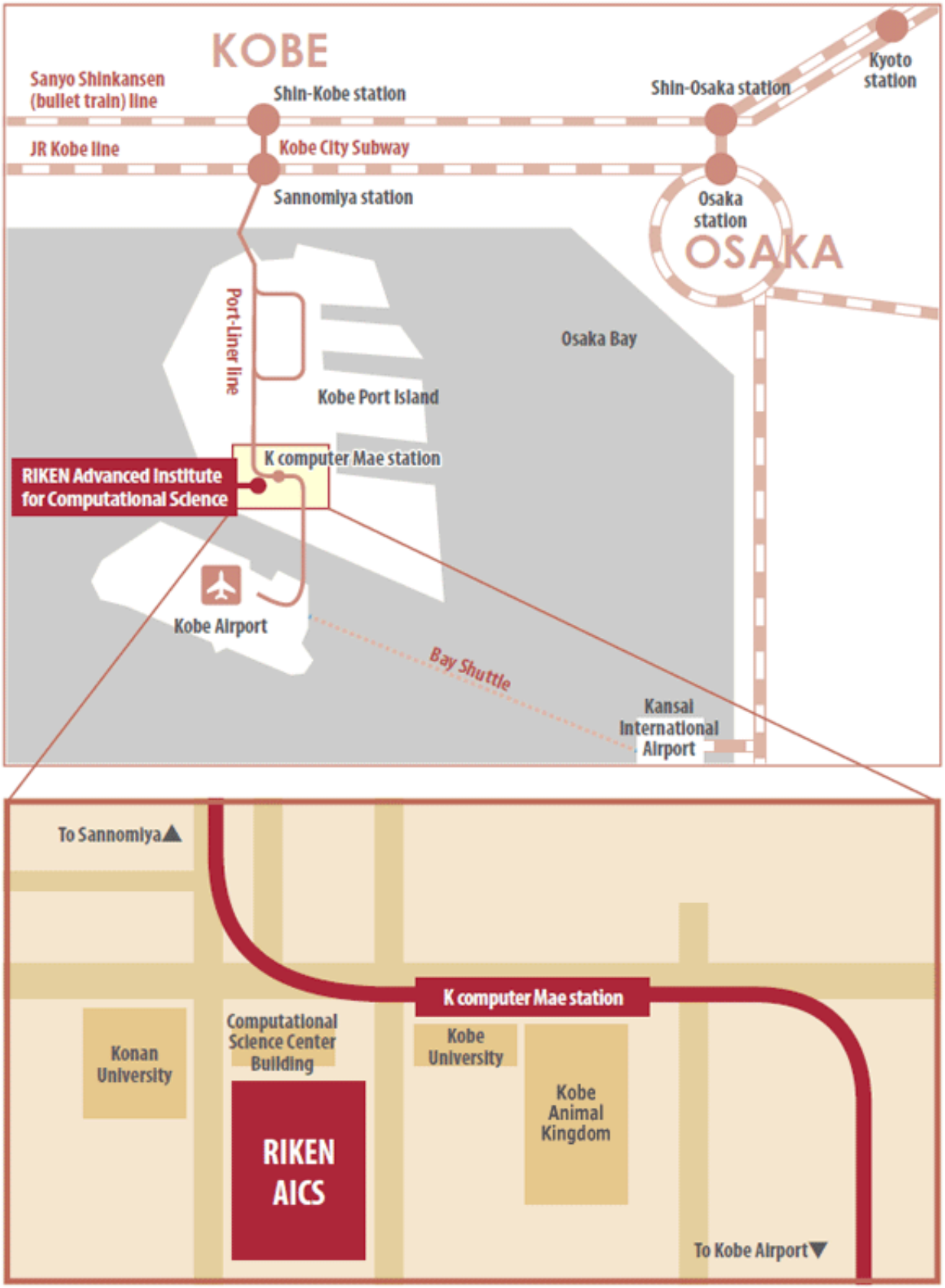
1st floor



6th floor



Area Map


KOBE
Sanyo Shinkansen (bullet train) line
Shin-Kobe station
Shin-Osaka station
Kyoto station
JR Kobe line
Kobe City Subway
Sannomiya station
Osaka station
OSAKA
Port-Liner line
Osaka Bay
Kobe Port Island
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