The Fifth
AICS International Symposium

Computer and Computational Sciences for Exascale Computing

December 8–9, 2014, Kobe, JAPAN

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The Fifth
AICS International Symposium

Computer and Computational Sciences for Exascale Computing

Invited Lecture Program

December 8 (Monday)

Reception

09:30

Opening Session

10:00 – 10:10 Opening Address
Akira Ukawa
(RIKEN Advanced Institute for Computational Science)

10:10 – 10:30 Overview of AICS in 2014
Akinori Yonezawa
(RIKEN Advanced Institute for Computational Science)

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Chair Nobuyasu Ito, Makoto Tsubokura (RIKEN AICS)

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11:15 – 12:00 **World record of Graph500**
Koji Ueno 13
(Tokyo Institute of Technology)

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- Lunch boxes available on the 1st floor
- 13:00 – 13:30 K-tour

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Poster Session Program

Invited Lecture

December 8 (Monday)

Speakers List

Yutaka Ishikawa

Koji Ueno

Michele Casula

Alexander Weiss

Yutaka Nakatsuka

Kizashi Yamaguchi

Simon Portegies Zwart

Kohei Murotani

Masaki Iwasawa

Development of Post K supercomputer

Yutaka Ishikawa
Project Leader, Exascale Computing Project
RIKEN AICS, JAPAN

The development of Post K supercomputer started in April 2014 as the Japanese FLAGSHIP 2020 project. The machine will be operated from 2020 to provide computational resources for scientists and engineers. Japanese government selected nine priority research areas and 5 frontier research areas that will be used in the Post K computer. The architecture of the Post K supercomputer is based on a general purpose manycore architecture, and it will be designed with the design of application and system software, so-called co-design of the system. By co-design, a more efficient execution environment than the K supercomputer will be carried out. A system software stack, such as OS kernel, communication and file I/O libraries is designed and developed not only for Post K supercomputer, but also for existing multicore/manycore architectures to bring the same software stack to commodity-based cluster systems.

World record of Graph500

Koji Ueno
Tokyo Institute of Technology, Tokyo, Japan

Graph500 is a new benchmark for supercomputers to complements the Top500 for large-scale data analysis problem. The ranking of Graph500 is based on the performance of large scale graph processing. The main kernel is Breadth-First Search (BFS), which is one of the most basic graph algorithms. Graph500 conducts BFS on a single large graph. Since the state of the art high performance supercomputers consist of large number of distributed memory machines, Graph500 requires efficient distributed parallel BFS algorithm.

However, efficient distributed BFS for large machines is a hot research topic and the best algorithm is not known. Furthermore, computing distributed BFS requires complex network communication and irregular memory accesses, which prevents the distributed parallel BFS from scaling to large machine sizes. Both developing efficient algorithm and architecture specific optimization is important to get high performance on Graph500.

We developed efficient scalable distributed BFS algorithm, 2D partitioning hybrid BFS, and achieved 17,997 GTEPS using 65,536 nodes. With this result, K computer is ranked No.1 on the June 2014 Graph500 List. Our current performance on K computer is 19,585 GTEPS submitted on November 2014 while the initial performance, which is submitted on November 2012, was 5,524 GTEPS. We present our efficient distributed BFS algorithm and the performance improvement on K computer. The current performance is brought by a sophisticated process distribution that is optimized for the K's 6D torus mesh network and increasing parallelism to hide the network latency and improve utilization of the network bandwidth.

Probing structural, magnetic, and superconducting properties of iron selenide (FeSe) by quantum Monte Carlo methods

Michele Casula
CNRS and Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Université Pierre et Marie Curie, 4 place Jussieu, 75252 Paris, France

In this talk we will illustrate how quantum Monte Carlo (QMC) simulations can shed light on the complex physics behind the iron based superconductors. Thanks to the computing power now available at the K and other high performance computers, it became possible to carry many-body QMC calculations out from first principles. We will discuss our present understanding of structural, magnetic, and superconducting properties of the FeSe iron selenide. We will address the interplay between magnetic fluctuations and structural properties in the FeSe phase diagram. The QMC optimized geometry is in good agreement with experiment without imposing a long-range spin order, thus solving a puzzle present since the earliest density functional theory calculations of this material. By symmetry arguments, we demonstrate that the electronic pairing in iron-based high-temperature superconductors shows a structure which is a linear combination of planar s-wave and d-wave symmetry channels, both preserving the 3-dimensional A1g irreducible representation of the corresponding crystal point-group. We provide evidence of these general properties by performing accurate QMC ab-initio calculations of the pairing function in FeSe. Our theory can rationalize and explain a series of contradictory experimental findings, such as the observation of twofold symmetry in the FeSe bulk superconducting phase, and nodeless gap in FeSe monolayer.

The kernel polynomial method and its applications

Alexander Weisse
Max Planck Institute for Mathematics, Bonn, Germany

Efficient and stable algorithms for the calculation of spectral quantities and correlation functions are some of the key tools in computational condensed-matter physics. I will give a short review of algorithms based on Chebyshev expansion and of the kernel polynomial method, which usually scale linearly with the problem dimension. The capacity of these methods will be illustrated with examples from the fields of disordered systems (densities of states, conductivities), electron-phonon systems, or quantum spin models (finite-temperature correlations). In addition, I will show how the kernel polynomial method can be embedded into other numerical techniques, e.g., Monte Carlo simulations.

Relativistic extension of quantum Monte Carlo method for atoms and molecules

Yutaka Nakatsuka
RIKEN AICS, Kobe, Japan

The Quantum Monte Carlo (QMC) method is a suitable method for massively parallel computation of electron-correlation effects in physical and chemical problems. While the target of molecular orbital theory or density functional theory has been extended to systems including heavy elements, the QMC method has been limited to systems with light elements. To treat molecular systems with heavier elements, the inclusion of relativistic effects – scalar relativistic and spin-orbit effects – is required.

To treat the scalar relativistic effect, we have developed relativistic quantum Monte Carlo methods based on the zeroth order regular approximation (ZORA) Hamiltonian, whose kinetic term is suitable for the real space MC integration. The scalar ZORA QMC method includes three extensions to the nonrelativistic QMC method – (1) the ZORA local energy expression, (2) the ZORA cusp correction scheme, and (3) the ZORA approximate Green's function. The developed methods are implemented in "R4QMC", a QMC program of "NTChem" software developed for the K computer. The details of theory and implementation of the relativistic extension of the QMC methods for general molecular systems are presented.

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[2] Y. Nakatsuka, T. Nakajima, and K. Hirao, J. Chem. Phys. 132, 174108 (2010).
[3] Y. Nakatsuka, and T. Nakajima, J. Chem. Phys. 137, 154103 (2012).

Magneto-structural correlation on the $CaMn_4O_5$ cluster in the oxygen evolving complex of photosystem II

Mitsuo Shoji,[a] Hiroshi Isobe,[b] Shusuke Yamanaka,[c] Jian-Ren Shen,[b]
Nobuo Kamiya,[d] and Kizashi Yamaguchi,[b,c,d]
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[d]*Osaka City University*, *Osaka*, *Japan ;* yama@chem.sci.osaka-u.ac.jp

Photosystem II (PSII) is the only known biological system that as the unique capability of utilizing visible light for the oxidation of water molecule into molecular oxygen as shown in eq. (1): $2H_2O \rightarrow O_2 + 4e^- + 4H$ [1]. This water splitting reaction is catalyzed with the Ca-doped Mn_4 oxide cluster ($CaMn_4O_5$) in the oxygen evolving complex (OEC) of PSII. Here, large-scale quantum-mechanical (QM)/molecular mechanics(MM) calculations have been performed to elucidate magneto-structural correlations on the $CaMn_4O_5$ cluster in OEC of PSII [2-8]. A high-resolution x-ray structure determined by Shen, Kamiya and co-workers in 2011 [1] was used as the initial structure for the QM/MM geometrical optimizations [4]. The optimized Mn-Mn and Ca-Mn distances by QM/MM are consistent with the EXAFS values by Berkeley group. The fully optimized geometries by QM/MM have revealed the structural symmetry breaking (SSB) of the Mn_a-$O_{(5)}$-Mn_d bond in the $CaMn_4O_5$ cluster of OEC of PSII. The QM/MM calculations have also elucidated effective exchange interactions (J) between Mn ions in the clusters [3]. The exact diagonalizations of the Heisenberg model based on the ab-initio J values provided the projection factors for the ground and lower-lying excited states that were used for assignments of the EPR spectra available in the S_1, S_2 and S_3 states of PSII [8]. The spin coupling schemes were directly related to the local singlet diradical (LSD) mechanism for the O-O bond formation in water oxidation. The spin Hamiltonian models were useful for elucidation of similarities between native and artificial water oxidations [5,7]. Implications of the computational results are discussed in relation to design of artificial catalysts for water oxidation.

References:

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The reproducibility of scientific results by numerical computations

Simon Portegies Zwart
Leiden University, Leiden, Netherland.

The conservation of energy, linear momentum, and angular momentum are important drivers of our physical understanding of the evolution of the universe. These quantities are also conserved in Newton's laws of motion under gravity. Numerical integration of the associated equations of motion is extremely challenging, in particular due to the steady growth of numerical errors (by round-off and discrete time-stepping and the exponential divergence between two nearby solutions. As a result, numerical solutions to the general N-body problem are intrinsically questionable. Using brute force integrations to arbitrary numerical precision we demonstrate empirically that ensembles of different realizations of resonant three-body interactions produce statistically indistinguishable results. Although individual solutions using common integration methods are notoriously unreliable, we conjecture that an ensemble of approximate three-body solutions accurately represents an ensemble of true solutions, so long as the energy during integration is conserved to better than 1/10. We therefore provide an independent confirmation that previous work on self-gravitating systems can actually be trusted, irrespective of the intrinsically chaotic nature of the N-body problem.

Zoom up tsunami analysis with many floating objects on urban areas by three analyses stages using distributed parallel explicit MPS method

Kohei MUROTANI and Seiichi KOSHIZUKA
Department of Systems Innovation, School of Engineering, the University of Tokyo, Tokyo, Japan

Ishinomaki city was severely damaged by the tsunami of the Great East Japan Earthquake two years ago. Our target is to simulate impact by the tsunami run-up with many floating objects on a seacoast and an urban area of Ishinomaki. Zoom up analysis by three analyses stages is adopted to solve a large area from an epicenter to an urban area.

In the first stage, the 2-dimensional viscous shallow water analysis is solved in the area of 667km×525km from the epicenter to the seacoast. In this analysis, the 2D mesh of 125m element size is used. In the second and third stages, the 3-dimensional tsunami run-up analyses are solved for the seacoast area of 10.5km×10km and the urban area of 660m×810m, respectively, using the parallel explicit MPS (Moving Particle Simulation) method. In the second stage, 130 million particles of diameter 2m are used. In the third stage, 400 million particles of diameter 0.3m are used and 431 floating objects flow in the urban area. In this research, the weak coupled problem by interplay between rigid bodies and fluid is solved for the flow of the floating objects.

For solving these tsunami run-up analyses, a new distributed memory parallel algorithm of the explicit MPS method has been developed. An analysis region of this method is divided for a distributed memory parallel computation using ParMETIS. These analyses have been carried out on the supercomputer FX10 and CX400 of the University of Tokyo, Kyushu University and Nagoya University.

FDPS: Framework for Developing of Particle Simulators

Masaki Iwasawa
RIKEN AICS, Kobe, Japan

Particle simulations are widely used in many fields of science and engineering. Examples include gravitational or molecular dynamics N-body simulations, fluid simulations by SPH or MPS, and granular simulations. Many researchers in many fields have developed software for particle simulations more or less individually. The algorithms used are largely similar. For example, some tree structure is used for interaction calculation and the neighbor search, and domain decomposition is used for parallelization on distributed-memory parallel computers. To develop an efficient program for particle simulation for large-scale parallel machines such as K computer is not easy, and to some extent the efforts of many very competent researchers, which could have been used to advance science, have been spent on the programming and tuning.

We are developing a framework which helps the researchers to develop efficient programs for particle simulation on large parallel machines, which we call Framework for Developing of Particle Simulators, or FDPS. The API of FDPS is given in C++. A user of FDPS need to provide the particle class and the function to evaluate particle-particle interactions. FDPS automatically decomposes domain, scatters particles and calculate interactions. The user program then integrates the orbits (and other physical quantities if necessary) of particles using the calculated interaction. Since the interaction calculation and relocation of particles are done in the FDPS part, there would be no need for the user to implement these complicated procedures, which we believe greatly improves the productivity of the researchers. In this presentation, we will overview the specification, the usage model, and the performance of FDPS.

Invited Lecture

December 9 (Tuesday)

Speakers List

Xuhui Huang

Sihyun Ham

Yasuhiro Matsunaga

Johan Hoffman

Ferenc Kun

Hiroshi Kawai

Niclas Jansson

Kohei Amano

Santo Fortunato

Yohsuke Murase

Takeshi Uchitane

Millisecond Molecular Dynamics of RNA Polymerase II Translocation at Atomic Resolution

Xuhui Huang
Department of Chemistry, The Hong Kong University of Science and Technology

Transcription, the synthesis of RNA from a complementary DNA template, plays a crucial role in cellular regulation, including differentiation, development, and other fundamental processes. We performed computer simulations to understand the thermodynamics of the major states of transcription elongation and the kinetics of transitioning between them for RNA polymerase II (pol II). In this talk, I will use pol II Translocation as an example. The main challenge for computer simulations is to reach biologically relevant timescales, which are orders of magnitude longer than most atomistic simulations. In order to overcome this timescale gap, we have applied Markov State Models to extract long timescale dynamics from short simulations. We reveal that RNA polymerase II translocation is driven purely by thermal energy and does not require the input of any additional chemical energy. Our simulations show an important role for the bridge helix: Large thermal oscillations of this structural element facilitate the translocation by specific interactions that lower the free-energy barriers between four metastable states. Among these states, we identify two previously unidentified intermediates that have not been previously captured by crystallography. The dynamic view of translocation presented in our study represents a substantial advance over the current understanding based on the static snapshots provided by X-ray structures of transcribing complexes.

Distinct role of water in protein-protein interactions

Sihyun Ham
Department of Chemistry, Sookmyung Women's University, Seoul, Korea

Understanding the molecular determinants of the relative propensity for proteins to aggregate in a cellular environment has been a central issue in attacking protein-aggregation diseases and in the development of human therapeutics. Despite the expectation that the protein aggregation can largely be attributed to the direct protein-protein interactions within an aggregate or in solution, we here unveil a crucial role of hydration water in ruling the aggregation propensity of proteins both in vitro and in vivo. The protein overall hydrophobicity, defined solely by the hydration free energy of a protein in its monomeric state sampling its equilibrium structures, was shown to predominantly dictate the protein aggregation propensity in aqueous solutions. We also find striking discrimination by the hydration water of positively and negatively charged residues depending on the protein net charge in regulating the solubility of a protein, which establishes novel design strategies for the biotechnological generation of aggregation-resistant proteins as biotherapeutics

Molecular Dynamics Simulation Studies Using Multi-Copy Based Methods: String Method and Sequential Data Assimilation

Yasuhiro Matsunaga
RIKEN AICS, Kobe, Japan

Conformational transitions of biomolecules are essential for the regulation of important chemical reactions in cells. Although all-atom molecular dynamics simulation is a powerful approach to investigate atomic details of biomolecular structure and dynamics, it is hard to access the time-scale of such slow transitions with conventional brute-force simulations. Recently, various methods using multi-copies of simulation system have been proposed to overcome the time-scale problem. In this talk, we will report our two on-going studies using such multi-copy based methods; string method, and sequential data assimilation. The string method efficiently searches the most probable pathway in conformational changes. We have applied the method to the drug extrusion process of multidrug efflux transporter AcrB. Our simulations show the importance of cooperative behavior in the transmembrane region and porter domain for the drug extrusion. The sequential data assimilation is a new approach in biomolecular simulations, which incorporates experimental data into simulations based on Bayesian statistics. We have developed the data assimilation framework for single-molecule FRET (smFRET) experimental data. Our test simulations show that the method can make robust estimates for latent conformational variables from smFRET photon-counting data.

High Performance Adaptive Finite Element Computation of Turbulent Flow and Fluid-Structure Interaction

Johan Hoffman
KTH Royal Institute of Technology, Stockholm, Sweden

Adaptive finite element methods (AFEM) using unstructured meshes pose serious challenges for the development of efficient algorithms and software implementations for massively parallel architectures. Here we present an AFEM framework for turbulent flow and fluid-structure interaction, based on a posteriori estimation of the error in target output, such as the drag of a car, or lift of an airplane. The error estimates are based on the solution of an adjoint (or dual) problem, which gives sensitivity information used to quantify the effect of local errors on the output of interest. The full AFEM algorithm thus calls for the solution of a primal problem, typically the Navier-Stokes equations, an adjoint problem, and the refinement of the finite element mesh. In the PRACE Tier-0 project FEniCS-HPC, this AFEM algorithm is implemented for the most powerful supercomputers in Europe, as part of the FEniCS open source project. The code show near optimal weak and strong scaling to tens of thousands of processing elements, and has been applied to simulate the turbulent flow past models of a car, airplane landing gears, and an airplane wing-body configuration. Biomechanics is another domain of application where FEniCS-HPC is used to model blood flow in the human heart, and the human voice organ. We will here present the methods, algorithms, and applications of AFEM with FEniCS-HPC.

Discrete element modeling of fracture and fragmentation phenomena

Ferenc Kun
Department of Theoretical Physics, University of Debrecen, Debrecen, Hungary

Discrete element modeling (DEM) is one of the most efficient computational approaches to the fracture processes of heterogeneous materials on mesoscopic scales. From the dynamics of single crack propagation through the statistics of crack ensembles to the rapid fragmentation of materials DEM had a substantial contribution to our understanding over the past decades.

We give a brief overview of the method and focus on two fields of application where DEM played a decisive role to achieve recent success: Computer simulation of the fracture of sedimentary rocks were carried out to investigate the emergence of crackling noise, i.e. sudden outbreaks of local micro-fractures that generate acoustic emissions. Studying the statistics of crackling events, correlations of their characteristic quantities, and the spatial structure of damage made it possible to identify precursors of the imminent catastrophic failure that is promising for developing forecasting methodologies. Energetic loading of a solid generates the simultaneous evolution of a large number of cracks which leads to a rapid breakup into small pieces. DEM simulations of fragmentation processes of heterogeneous materials induced by various different types of loads helped to clarify the origin of the universality of fragment mass distributions observed throughout in nature and in experiments.

Finally, recent applications of DEM will be presented on the damage and rupture of biological systems such as the human head induced by different types of mechanical loading that occur e.g. in car accidents.

Implementation of Domain Decomposition Method on open-source CAE system ADVENTURE

Hiroshi Kawai
Tokyo University of Science-Suwa, Nagano, Japan

Performance tuning approaches of a structural analysis code based on the domain decomposition method (DDM) for peta-scale massively parallel supercomputers are presented. First, a new subdomain local finite element solver, DS-LSC, using explicit evaluation of local Schur complement, is introduced. Next, the coarse grid correction step in BDD pre-conditioner is accelerated by the explicit evaluation of the inverse of the coarse matrix. These approaches are effective for a linear dynamic analysis, where a linear equation with the constant coefficient matrix has to be solved repeatedly. About 10 % of peak FP performance is obtained on RIKEN K Computer using 32768 nodes. The implementation will be introduced to the future version of open-source CAE system, ADVENTURE, and it will be utilized for huge-scale seismic analysis of a nuclear power plant.

Introduction of Complex Phenomena Unified Simulation

Niclas Jansson
RIKEN Advanced Institute for Computational Science

Writing high performance scientific software is a delicate task. These codes are often developed on an application to application basis, highly optimized to solve a certain problem. For coupled simulations, different solvers have to be used and interfaces between the different components have to be developed, which makes optimization of the entire application a challenge. In this talk, we present our work on developing a unified simulation method that map all discretized equations onto the same grid and solve the coupled problem as a unified continuum. To address the challenges of modern and emerging supercomputers, efficient data structures and parallelization methods are needed. Here, we use the Building Cube Method (BCM), a hierarchical Cartesian grid with an immersed boundary method to accurately capture complex geometries, while still achieving an underlying data structures that are both cache and SIMD friendly. Since computation can be carried out on each cube independently, BCM allows for an efficient parallelization with low communication costs that can scale to hundreds of thousands of cores. Enabling efficient time resolved simulations of industrial multiphysics problems.

Design optimization method for vehicle body structure developments

Kohei Amano
Technical Research Center, Mazda Motor Corporation,
Hiroshima, Japan

Growing demand for light-weight vehicle has become a big challenge to reduce CO_2 emissions for global warming. Simulation technology to estimate lightest body structure while maintaining vehicle attributes such as crashworthiness, handling performance, aerodynamics etc. have been strongly required in vehicle body development process. Multidisciplinary design optimization method has been developed in order to solve this issue. It has been implemented in the process and allows engineers to produce light-weight and good performance vehicle body design.

This optimization method, attribute analysis simulation methods and status of application of simulation tools to vehicle body development process will be presented. Future development plans regarding coupled analysis for multi attributes and optimization for multi vehicle bodies considering the super computer in practical use will be presented as well.

Scaling and universality in collective social phenomena

Santo Fortunato
Aalto University, Espoo, Finland

The availability of big datasets on social phenomena has opened new exciting perspectives for researchers. Especially the Web, with its jungle of social Websites and data repositories, has transformed the way we study social behavior at all scales, leading to the new discipline of computational social science. Large numbers enforce the adoption of statistical techniques, aiming at the identification of regular patterns from the apparently erratic behavior of single individuals.

The concepts and techniques of statistical physics have proven to be very helpful to uncover and understand such regularities in collective social behavior. Here I will give two examples of social phenomena exhibiting scaling and universality, alike critical phenomena in physical systems. I will show how, after suitable normalization, the performance of candidates in proportional elections and of scientific papers, measured by the number of votes and citations, exhibit universal distributions, regardless of the country where the elections was held and the topic of the paper.

Such examples indirectly confirm the social atom hypothesis, i.e. the emergence of regular collective behavior from local interactions between people, regardless of peculiar details of the individuals.

Multi-Layer Weighted Social Network Model

Yohsuke Murase
RIKEN Advanced Institute for Computational Science, Kobe, Japan

The abundance of data due to the rapid development of the information and communication technology (ICT) has generated entirely new, multidisciplinary approaches in social sciences, in which network theory and computational science play a considerable role both in terms of data analysis and modeling. One of the major challenges in this context is the understanding of the structure of the society, which is crucial for many applications ranging from epidemiology to urban planning.

Among a broad range of ICT data, mobile phone data have a special role in this endeavor as much of the inter-personal communication runs today over mobile phones. Various analyses on this mobile call network have revealed the characteristics of social networks such as the Granovetterian structure, modular topology, and spatial patterns.

In this talk, we are going to present our research aiming at constructing a model for a weighted and multi-layer network which reproduces some of the important structural features of the mobile phone dataset. Since a naive introduction of multiple layers breaks the Granovetter-type weight-topology relation, we introduced an extension such that each node has a geographic position and that geographically close nodes have more chance to form a link. The extended model successfully fulfills the requirements, and shows the importance of geographic correlations in multi-layer social networks.

OACIS - A tool for social simulation execution and its applications

Takeshi Uchitane
RIKEN, Kobe, Japan

Social simulations generally have various parameters. This is because that model of social phenomena becomes so complex in considering many factors. Moreover, social simulations generate multiple results on a single run. This is because social phenomena are evaluated from various perspectives. In order to get an insight from social simulations, it is expected to perform comprehensive numerical simulation on a supercomputer since the number of scenarios gets larger as the number of simulation factors and evaluation perspectives increases. However, when social model inputs and outputs are analyzed, e.g. classification of the results or finding the critical points of phase transitions, researchers must select simulation scenarios to make a data set for the analysis since it is impossible to perform simulation jobs for whole scenarios even if researchers can use super computers. Requirement of the scenario selection is the reason why researchers need to prepare simulation jobs and to gather the simulation results many times. However, it is too hard to handle huge numbers of simulation jobs manually and it is also too hard to gather dynamically generated results manually.

In Discrete Event Simulation Research Team, RIKEN, a tool helps researchers handle a lot of simulation executions and gather simulation results is developed. The tool is named “Organizing Assistant for Comprehensive and Interactive Simulations” (for short OACIS) and OACIS has been released as an open source software under the term of the MIT license. OACIS has some features to help researchers analyze social models. For example, OACIS can submit simulation jobs, monitor them and store results into appropriate directories automatically. On the other example, OACIS can gather dynamically generated results in the same manner. In presentation, we also show an analysis of vehicle traffic simulation as an application of OACIS and we will discuss a development road map of OACIS.

Poster Session

December 8 and 9
(Monday and Tuesday)

1P

The Multi-GPU Implementation for Natural Convection Problems with Multiple Open Boundaries

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Natural convection in parallel squares plats with a heated bottom surface is investigated numerically. For solving the open boundary problems of natural convection, the hybrid boundary condition is adopted as a non-reflection boundary condition. Methods of the Roe scheme, preconditioning and dual time stepping matching the DPLR scheme are used to solve low speed compressible flows. The Multi-GPU implementation by the CUDA computing platform is investigated and compared with the OpenMP method. The results show that the performance of two Nvidia GTX Titan is about 20 times more than the Intel Core i7 4930K in parallel computation.

2P

Large-scale integrated models of basal ganglia-thalamo-cortical circuit toward reproducing Parkinson's symptoms

Jan Moren, Jun Igarashi, Junichiro Yoshimoto and Kenji Doya

Okinawa institute of Science and Technology

Tremor is a debilitating side effect of Parkinson's disease. It likely originates in neural cell interactions between the STN and GPe in the basal ganglia, but its propagation and final physical manifestation involves large parts of the CNS motor areas, the descending pathways and physical muscle characteristics.

To better understand this symptom, we need a system-scale model of those motor systems that are primarily implicated in Parkinsonian tremor. That includes the motor cortex, thalamus and basal ganglia as well as spinal cord and muscle models. A single model encompassing all these components is infeasible, so we develop them as separate models that are interconnected at runtime. We have used smaller models of these areas to verify the feasibility of connecting multiple separate models and running them together in a cluster. Now we are developing the full-scale models.

The motor cortex and thalamus are modeled as a 3D neural circuit, corresponding to 1.2x1.2 mm^2 cortical surface. The model consists of about 91K cortical neurons and 5K thalamic neurons. The motor cortex has laminar structure consisting of layers 1, 2/3, 5A, 5B, and 6. Each layer has excitatory and inhibitory cells. The thalamus consists of two sub-regions. The model represents multiple cortical columns that process different motor behaviors. Lateral inhibition between columns activates only target motor behaviors.

The basal ganglia is modeled as rat-scale 2D layers. The striatum is scaled in proportion to the cortex; the full-size striatum has ~2.8M medium spiny neurons, whereas a 1.2×1.2mm^2 cortical slice corresponds to ~80K MSN. The other areas are far smaller than the striatum, so we model them at full size. The GP/GPe is 2.6×1.6mm with 46K neurons; the STN is 1.08×0.88mm with 13.6K neurons and the EP/GPi will have 3.2K neurons.

We will show the resulting model architectures and discuss their interconnections.

3P

GPM/DPR Precipitation Compared with a 3.5-km-resolution NICAM Simulation

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This poster presents our recent paper accepted by Scientific Online Letters on the Atmosphere (SOLA). In February 2014, the Global Precipitation Measurement (GPM) satellite was launched successfully and started observing global precipitation using the new DPR (Dual-frequency Precipitation Radar) sensor. This study pioneers to compare the GPM/DPR precipitation products with other satellite-derived products and simulated precipitation from the Nonhydrostatic Icosahedral Atmospheric Model (NICAM) at a 3.5-km horizontal resolution. The NICAM simulation outputs are converted to three-dimensional radar reflectivity using a radar simulator included in the joint simulator for satellite sensors (Joint-Simulator). We focus on the three frontal precipitation cases in the storm track regions, where the NICAM surface precipitation agrees generally well with an existing precipitation product "GSMaP". The surface precipitation patterns, bright band heights and three-dimensional radar reflectivity of GPM/DPR generally agree with the corresponding variables from GSMaP, NICAM and the Joint-Simulator. However, the radar echo tops of GPM/DPR are systematically lower than that of NICAM-Joint-Simulator, suggesting that NICAM may overestimate mixing ratios of snow and graupel. The general agreement of surface precipitation patterns between GPM/DPR and the NICAM simulation encourages a possible use of GPM-derived precipitation data toward numerical weather prediction through data assimilation.

4P

Anisotropic crack patterns induced by memory effect of paste

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A densely packed colloidal suspension, called paste, remembers the direction of its motion, such as vibration and flow, due to its plasticity. The memory of such motion can be visualized as a morphology of desiccation crack patterns. When a water-poor paste is vibrated, the paste remembers the direction of the vibration even after the vibration stops, and desiccation cracks run in the direction perpendicular to the direction of the initial vibration. On the other hand, when a water-rich paste is vibrated, the paste flows, and once the paste flows, it comes to remember its flow direction, and the desiccation cracks run in the direction parallel to the direction of the initial flow [1-2].

A residual tension theory is presented to explain memory effect of vibration. It is demonstrated that the horizontal oscillation can produce residual tension in the paste layer, modeled as a shallow-water-like system of elasto-plastic fluid, if the non-uniformity or the nonlinear effect of the deformation is taken into account [3-4]. As for a memory of flow, interparticle interaction is found to play important roles [5]. It is shown that memory effect of paste can be applied to produce various types of desiccation crack patterns, such as cellular, radial, lamellar, spiral and ring, by imprinting any flow patterns into pastes [1-2, 5].

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5P

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

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Water birds such as shorebirds and waterfowl breed in the Arctic tundra. Therefore, the vegetation shift from tundra to taiga due to climate change must be one of the most important habitat changes for water birds. To simulate the Arctic vegetation shift and to evaluate its impact on water bird breeding, we are developing an ensemble data assimilation system with a dynamical global vegetation model known as the SEIB-DGVM (Spatially -Explicit-Individual-Base Dynamic-Global-Vegetation-Model). As the first step, data assimilation experiments were performed with the SEIB-DGVM using simulated LAI observations. The results suggest that the LAI is a key to designing an appropriate data assimilation system for the SEIB-DGVM.

6P

Short term forecasting for precipitation by utilizing a new three-dimensional super-rapid phased array weather radar data

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Short-term precipitation forecasting (a.k.a. nowcasting) is important for navigating meteorological disasters such as typhoons and severe storms. Conventional nowcasting approaches are based on two-dimensional five-minute-scan radar data which may limit their forecasting accuracies due to the difficulties in capturing a rapid development of convections. In this study, a 3-D precipitation extrapolation system is developed using the latest phased array weather radar (PAWR) which is capable of a 100-m resolution 3-D volume scan every 30 seconds. First, motion vectors are estimated based on the COTREC algorithm using two consecutive radar scans. Second, the precipitation field is extrapolated with the motion vectors based on a weighted essentially non-oscillatory (WENO) scheme. The extrapolation system showed improved forecasting results with the super rapid 3-D PAWR data compared to its 2D counterparts.

Keywords: Nowcasting, phased array radar, Extrapolation.

7P

Temporal Parallel Approach to Configure Multiscale Simulations for Complex Phenomena

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Many attempts have been done to represent multiscale problems in various fields of science. They are successful to a certain extent within static representation of those systems, and are still studied extensively. Recently, several multiscale frameworks were proposed [1] to simulate dynamic properties of phenomena. Our approach is to apply these spatial and temporal multiscale methods to nonlinear phenomena, where the temporal parallel algorithm [2] is used as a higher-order perturbation to ensure sufficient accuracy [3].

Nonlinear phenomena observed in our daily life often contain multiple scales of dynamics: a fractal pattern on the top of a milk cup [4] (Fig.1) is created by viscous fingering within a thin film on the surface and is influenced by three-dimensional convection; complex dynamics in air-reed instru- ments [5] (Fig.2) are induced by interaction between sound and fluid. In order to study these complex phenomena, it is necessary to combine minimum models for essential understanding and simulations for precise reproduction. Thus, effective ways to configure multiscale simulations to describe complex phenomena are desired. In this poster, numerical approaches for multiscale phenomena are presented with the temporal- parallel method. It is also discussed how to configure effective representation for those multiscale problems.

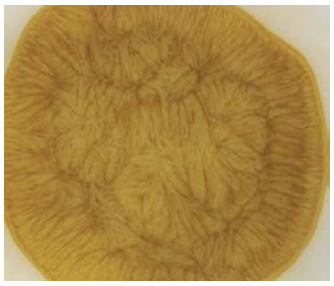

Fig.1 Coffee fractals

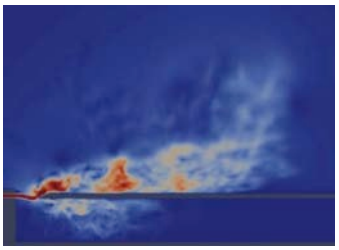

Fig. 2 Air-reed instruments

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8P

Ensemble data assimilation for a large parallel numerical weather prediction model: Development of the SCALE-LETKF syste

Guo-Yuan Lien, Takemasa Miyoshi, Seiya Nishizawa, Hisashi Yashiro, Ryuji Yoshida, and Hirofumi Tomita

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Numerical weather prediction (NWP) models have been run in large parallel computing machines. Meanwhile, ensemble weather forecasts and ensemble data assimilation, which require simultaneously running tens of copies of the NWP models, have also been useful and routine tasks in the field of NWP. Therefore, running an ensemble of large parallel NWP models has become a necessity. Ideally, running independent ensemble members in perfectly parallel would be easy and straightforward. However, if one wants to perform ensemble data assimilation as well as the ensemble model simulations, more sophisticated design would be needed in order to be applicable to large systems. The NWP models are parallelized by splitting their simulation domains into subdomains, but the ensemble data assimilation is usually more easily parallelized by splitting the calculation over the ensemble space. Therefore, without a careful design most of the computation time could be wasted in the node-to-node communication and data I/O processes.

We have been developing the SCALE-LETKF system that couples a highly parallelized large-eddy-simulation weather model with an ensemble data assimilation method, the local ensemble transform Kalman filter (LETKF). The targeted goal is to conduct rapid update cycle data assimilation at very high resolution using this system. In order to meet the goal, we propose changes of the data I/O flow and the parallelization scheme of the LETKF program in order to improve its parallelization efficiency and scalability for very large problems. The concept of the parallelization strategy and the results from the preliminary version of the SCALE-LETKF system will be presented in this poster.

9P

The 10,240-member ensemble Kalman filtering with an intermediate AGCM without localization

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AICS Data Assimilation Research Team

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. In this study, we increase the ensemble size up to 10,240, much larger than the typical choice of about 100, and remove the localization completely in an EnKF. The 10,240-memeber EnKF is implemented with an intermediate AGCM known as the SPEEDY. A 1-month data assimilation experiment under the perfect model scenario is performed, and longer-range error correlations and non-Gaussianity are investigated. The results show that the 10240-member EnKF without localization provides very accurate analysis, and if we apply 2000-km localization (more than 7000-km radius of influence), the analysis is significantly degraded. Namely, the 10000-km scale error correlations in the 10240-member EnKF actually help improve the analysis.

10P

The solvent-accessible surface area of proteins affects water structure and dynamics

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Recently the static structure and the dynamic behavior of water in crowded environment have been shown significantly affected by the protein crowders, as a function of protein volume fraction. In this study, using molecular dynamics (MD) simulations we found that the solvent-accessible surface area (SASA) of proteins in a crowded environment has a substantial effect on the structure and dynamics of water, even at the same protein volume fraction. A series of chicken villin headpiece, protein G, and bovine serum albumin (BSA) systems were built and each was simulated for 50 ns. Hydration structure was analyzed in terms of solvent-accessible volume, percentage of water location, radial distribution functions, and coordination numbers. Water dynamics was analyzed using self-diffusion coefficients and dielectric constants as a function of total SASA. The results show that the water structure and dynamics were altered differently in each system. The diffusion of water is also significantly reduced and shows a linear trend as a function of total SASA. The change in the water dynamics can be related to the ratio of water in the bulk region. The results suggest a novel view on the protein crowding effect on hydration.

11P

Convective-scale predictability in numerical weather prediction at a 100-m resolution

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Recent developments in high-performance computing and advanced observing technologies enable us to step forward to cumulus-convective-scale data assimilation for numerical weather prediction at a horizontal resolution of O(100) m, O(10) times higher than the previous studies (e.g., Leoncini et al. 2010; Melhauser and Zhang 2012; Keil et al. 2014). Understanding the predictability of convective-scale weather plays an essential role in designing such high-resolution numerical weather prediction systems. In particular, it would be important to know what would be the effective temporal frequency of data assimilation, whether or not it needs to be the order of seconds. This study performs 30-second breeding cycles at a 100-m resolution using the Weather Research and Forecasting (WRF) model, and explores the convective-scale predictability.

The results of breeding experiments show that bred vectors develop around the edge of newly developing convective cores and spread away from the convective cores. Different rescaling intervals with the same rescaling value show similar spatial structures of the bred vectors. By contrast, different rescaling values produce different spatial structures.

12P

Performance evaluation of the EigenExa dense eigensolver on the K computer

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Solving real symmetric dense eigenvalue problems is one of the fundamental matrix computations required in many fields such as computational chemistry and data analysis. Currently, it is consensus that the widely-used ScaLAPACK library can hardly exploit the performance of petascale systems such as the K computer. A new library that are more suitable for such systems is thus strongly needed, and several projects that aim at developing it are ongoing (e.g. ELPA and DPLASMA). Also in Japan, a new dense eigensolver, named EigenExa, has been developed mainly by the second author. The EigenExa library employs an algorithm in which the eigenvalue problem of a banded matrix is directly computed without traditional tridiagonalization. This approach has not been practically used yet as far as the authors know.

In this poster, we mainly present the performance of the current EigenExa library. We evaluated EigenExa by using over 10,000 nodes of the K computer and compared it with ScaLAPACK. In our evaluation, EigenExa well scales and outperforms ScaLAPACK. We also introduce the features of EigenExa, particularly focusing on the differences from other libraries, and give our perspective on the further development of EigenExa for post-petascale systems.

13P

Replica State Exchange Metadynamics

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Metadynamics (MTD) is an enhanced sampling algorithm applicable for the computational studies of biosystems with high energy barriers and slow modes of motion. It based on a history-dependent bias potential in a collective variable (CV) space. In particular, we are focused on multireplica approaches such as the bias exchange MTD (BE-MTD), where the CV space is divided into lower dimensionality subspaces for efficiency and scalability.

We demonstrate that BE-MTD can be improved (shorter simulation times are required for the same accuracy) by replacing Metropolis-Hastings algorithm with advanced replica exchange schemes. The new proposed method is called replica state exchange metadynamics (RSE-MTD).

14P

30-second-update ensemble Kalman filter experiments using JMA-NHM at a 100-m resolution

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Local severe rainstorms may cause serious damage such as flooding and landslide, but its precise simulation is difficult mainly due to limited spatial and temporal resolutions of numerical weather prediction (NWP). To tackle this challenge, a 100-m-resolution NWP system is designed, so that the forecasts are updated every 30 seconds by assimilating observational data from the phased array weather radars (PAWR) at Osaka and Kobe. In addition, the next-generation geostationary satellite Himawari-8 will have a 30-second scanning mode for a limited domain, and using the Himawari-8 data is within the scope. An observation operator and quality control algorithm are developed for PAWR, and data assimilation experiments using the Local Ensemble Transform Kalman Filter (LETKF) are performed for the local heavy rainfall case that caused a disaster in Kyoto on 13 July 2013. In this presentation, a brief introduction to the experiments and the results will be presented.

15P

Block BiCGStab for lattice QCD on the K computer

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We have developed a block version of the Bi-Conjugate Gradient Stabilized (BiCGStab) solver for treating the Wilson-Dirac equation with multiple right-hand sides in lattice QCD with clover fermions. We implement the QR decomposition, Lüscher's domain decomposition Schwarz alternating procedure (SAP) preconditioner and the symmetric successive over-relaxation (SSOR) iteration with *locally lexicographic* ordering for obtaining the domain inverse. Code development and optimization are carried out for the K computer at the RIKEN Advanced Institute for Computational Science. The computation kernels have been shown to improve in performance depending on the SAP block size, the number of compute nodes, and the number L of right-hand sides. The block BiCCStab solver, written in single precision, will be included as a preconditioning step for an outer BiCGStab solver in double precision. Test calculations will be performed with lattice size 96^4, using 2048 nodes of the K computer. The computational cost is found to reduce with increasing the number L of right-hand sides up to ~20%. The performance of a computational kernel exceeds 50% efficiency, and the single precision block BiCGStab has more than ~30% sustained efficiency.

16P

All-atom Molecular Dynamics Simulation of the Complete Model of Bacterial Cytoplasm

Isseki Yu[1], Takaharu Mori[1], Jaewoon Jung[2], Tadashi Ando[3], Ryuhei Harada[2], Michael Feig[4], and Yuji Sugita[1,2,3]

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Understanding the dynamics and interactions of all biomolecule components in cell with atomic resolution is straightforward pathway that connect structural biology and systems biology. For this purpose, we constructed full atomistic model of the cytoplasm of bacteria (Mycoplasma Genitalium) with all of the molecular components, i.e., proteins, RNA, metabolites, ions, and solvent, that are mapped on the complete biochemical pathways. The size of the system is 100 nm x 100 nm x 100 nm, which is greatly exceeds that of typical molecular dynamics (MD) simulations, covering about 10% of the volume of an entire cell. Using the atomic trajectories generated by highly parallelized MD program GENESIS on K computer, influence of the cellular environment on the structure, enzyme activity, and dynamic properties of macromolecules and metabolites are analyzed. Furthermore, interactions between macromolecules and their correlation with biochemical reaction network are also discussed.

17P

Macromolecular dynamics in intracellular environment: Brownian dynamics simulation study

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One of the most characteristic features of the cellular interior is crowding. How does the crowding alter dynamics of macromolecules? By employing Brownian dynamics (BD) simulations of a coarse-grained (CG) model, we try to elucidate the principles of intermolecular dynamics in the crowded environment of cells. We first developed a parallelized BD algorithm that can rigorously handle hydrodynamic effects between particles. Next, we built a CG model of a *Mycoplasma genitalium* cytoplasm, where macromolecules are represented by spherical objects with their Stokes radii. Using the CG system and algorithm, long-time BD simulations were performed. In the meeting, we discuss these simulation results

18P

Development of High Performance Parallel Real Random Number Generator KMATH_RANDOM

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We develop a high performance parallel real random number generator, called KMATH_RANDOM for highly parallel computers such as K computer. KMATH_RANDOM can be applied for Monte Carlo simulations, visualizations, etc. In recent collaboration, a remote visualization system of 3D images 'PBVR' [1] successfully performs with KMATH_RANDOM.

KMATH_RANDOM is based on the open source real random number generator dSFMT [2] and is MPI parallelized. The KMATH_RANDOM library supports C, C++ and Fortran 90 interfaces, and is easy to integrate with parallelized simulation programs. Since KMATH_RANDOM maintains the runtime status files of the random number generator for each process, called 'jump files', users can easily restart and replay the simulation.

We have evaluated KMATH_RANDOM on K computer. The execution time to generate one billion real random numbers on 250 nodes (one process per node) of the K computer system is 0.20 seconds (excluding the time to generate jump files). It is 247 times faster than a conventional sequential Mersenne twister implementation (Boost ver. 1.53). The detailed results will be presented on the poster.

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19P

Computations on Optical and Electronic Vortices

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[2]*Dept. of Industrial and Management Eng., Sunmoon University, Korea*

The propagations of electromagnetic waves in the presence of electric space charges are one of key examples of light-electron interactions from a narrow viewpoint or field-matter interactions from a broader perspective. For large charge density and high wave intensity, the coupling between light and electrons is prohibitively nonlinear not to mention the many-body dynamics among electrons. Full quantum-mechanical approaches to both fields and electrons are often tried in recent days for nanoscopic systems. However, these approaches are not practical for mesoscopic systems due to computational over-burdens.

In this presentation, we will instead focus on the classical Maxwell's equations in the presence of space charges. In this case, we are faced with issues of modeling electric-current vectors in terms of electric charges and electromagnetic fields. This modeling should be not statically but dynamically adjusted depending on a particular problem at hand including a geometric configuration. For cylindrical geometry suitable for investigating optical vortices [1], we suggest some physically acceptable ways of properly modeling currents so that we could construct meaningful computational problems.

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When and how can evolving open systems grow?

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[2]*JST CREST* [3]*RIKEN AICS*

The stability/fragility of complex systems has attracted broad interest, especially since after the pioneering theoretical works in 1970s by Gardner, Ashby, and May. New insights have been brought, for example, from recent complex networks studies.

This talk reports a novel class of transition in the robustness of complex and OPEN systems. Openness is a key and universal feature of various real complex systems such as ecosystems, reaction networks in living organisms, economical systems, and social communities: their complexity emerges as a result of successive introductions of new elements.

Using an extremely simple model, it is found that systems under such open environment either grow toward infinitely large size or stay finite depending on the unique model parameter: the average number of interactions per element. Interestingly, this transition originates from the balance of the two effects: although having more interactions makes each element robust, it also increases the impact of the loss of an element. Compared with the classical condition for dynamical systems in which only one strong interaction per element is allowed, the condition for our different class of system to grow is far looser [1]. This newly discovered mechanism may provide us a most basic understanding on real complex systems.

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21P

Theoretical Study on Spin Forbidden Transition of Solar Cell Sensitizers: Two-component Relativistic Time-dependent Density Functional Theory Study

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Ru complexes have been demonstrated as a promising dye among solar cell materials. Recently, a phosphine-coordinated Ru(II) sensitizer, DX1 molecule, was reported to perform well as an organic photovoltaic material. The DX1 molecule has the feature that spin-forbidden singlet-to-triplet direct transitions occur because of the strong spin-orbit (SO) interaction, which indicates that the DX1 sensitizer can absorb long-wavelength lights through the spin-forbidden transitions and avoid energy loss originating from intersystem crossing. In order to examine the spin-forbidden transitions in details, we calculate the transition energies by two-component relativistic time-dependent density functional theory /Tamm-Dancoff approximation with SO interaction (SO-TDDFT), which was implemented into the quantum chemical program package, NTChem.

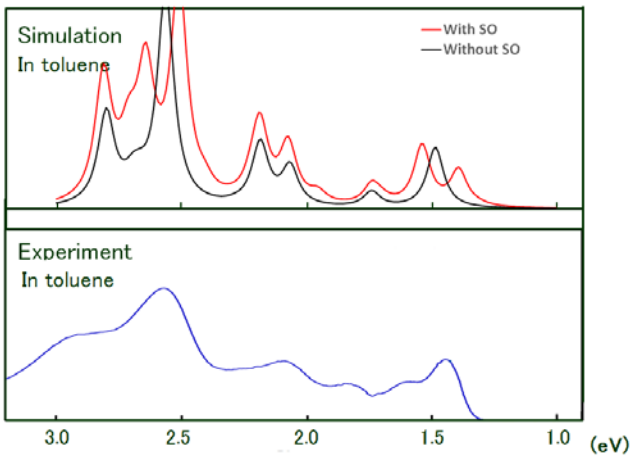

Figure 1. Absorption spectra of DX1 by experiments and by SO-TDDFT calculations with PBE1PBE. The basis sets used are Sapporo-DK-DZP and cc-pVDZ-DK for Ru and the others atoms, respectively.

The calculated absorption spectra of esterified DX1 molecule are shown with experimental one in Figure 1. The singlet-to-triplet transition around 1.35 eV, which is assigned to a metal-to-ligand charge-transfer type excitation, appears although it is slightly shifted to a lower energy in comparison with the experimental spectrum. The effect on the first peak from the SO interaction is large, whereas those on the other peaks are relatively small. The major peaks in the energy range from 1.5 to 3.0 eV are also reasonably reproduced. We also calculate DX1 derivatives that have different substituents and different central transition metals, and analyze the role of the substituents and why the central transition metal is Ru, not Fe and Os. The details will be given in the presentation.

22P

Massively parallel RI-MP2 energy gradient calculations on K computer

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RIKEN Advanced Institute for Computational Science

Second-order Møller–Plesset perturbation (MP2) theory is the simplest but robust electron correlation method to account for the non-covalent interactions that play important roles in the chemical phenomena of nano and biological molecules. In the case of geometry optimization, the $O(N^5)$ computational cost of the MP2 analytical energy gradient calculation becomes more serious problems than the MP2 energy calculation. To attain the geometry optimization calculation of the large nano and biological molecules at the MP2 level, the development of the efficient computational techniques for the MP2 energy gradient is desired.

We have developed a MPI/OpenMP hybrid parallel algorithm for the resolution of the identity MP2 (RI-MP2) energy gradient calculation and implemented into the NTChem software [1]. This algorithm is designed for the massively parallel calculations on the K computer. The loop of a virtual molecular orbital index is parallelized by MPI in the calculation of four-center two-electron integrals, one-particle density matrices, and two-particle density matrices to utilize more than a few thousand MPI processes. The RI-MP2/cc-pVTZ energy gradient calculation of buckycatcher $C_{60}@C_{60}H_{28}$ (3,992 AOs without the frozen core approximation) was successfully performed in 30 minutes using 4,096 nodes of the K computer. Using the new MPI/OpenMP hybrid parallel RI-MP2 energy gradient code, the MP2 geometry optimization of large molecules having up to 200 atoms and 5,000 AOs can be performed with high parallel performance and in modest time on the K computer.

[1] http://labs.aics.riken.jp/nakajimat_top/ntchem_e.html

23P

Assigning the 1800-3500 cm^{-1} Region of the Eigen Ion Vibrational Infra-Red Spectrum

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The assignments of vibrational infrared spectra are important for understanding the dynamics of both single molecules and clusters of molecules. The harmonic approximation often applied to this problem does not include important anharmonicities, often prevalent in loosely bound systems. This results in the dynamics of highly anharmonic motions being poorly or even wrongly described. Consequently anharmonic calculations are needed to describe the dynamics of molecular clusters accurately. The Eigen ion is a molecular cluster consisting of the hydronium ion (H_3O^+) and three water molecules. This is a system often associated with the dynamics of the solvated proton and can therefore help give insights into the dynamics of many important chemical and biological processes. We present the anharmonic spectra of the Eigen ion calculated using vibrational quasi-degenerate perturbation theory (VQDPT2) and a three mode coupled potential energy surface calculated at the B3LYP/aug-cc-pVTZ level. The calculated spectrum reproduces the experimental spectrum in the region 1800-3500cm^{-1} to a larger extent than previous studies. The spectrum in this region is believed to be a result of the internal dynamics of the solvated hydronium ion and its rotational motions when in solution. We provide a full analysis of the vibrational transitions in this region to support and extend this hypothesis.

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24P

Sphingomyelin clustering in three model lipid bilayers

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Theoretical Molecular Science Lab., RIKEN

Recent experimental evidence have suggested that sphigomyelin (SM) forms clusters in liposomes consisting of SM and DOPC (dioleoyl phosphatidylcholine) to which GFP-lysenin proteins can bind specifically, while these phenomenons are not observed in the liposomes consisting of SM and DPPC (dipalmitoyl phosphatidylcholine). Moreover, the Raman spectra of SM, SM/DOPC and SM/DPPC liposomes show significant difference in the intensity of the amide I stretching band (1600 to 1700 cm^{-1} region), indicating that the environment of the amide group of SM is different in these liposomes. However, the structure of the SM in these liposomes remains elusive. Here we perform a series of coarse-grained molecular dynamic simulations for the mix SM/DOPC and SM/DPPC bilayers and clusterize SM lipids based on the Voronoi diagram analysis. The phase segregation is observed in the SM/DOPC bilayer, but not in the SM/DPPC bilayer. Moreover, we perform a molecular dynamic simulation of SM/DOPC/cholesterol bilayer to study the cholesterol effect on the phase segregation. This study provides insight into the distinct SM cluster structure in these three mix lipid bilayers.

25P

Molecular Dynamics Simulations of the N1 Riboswitch Complexed with Aminoglycosides

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[3] *RIKEN, Japan*

Riboswitches are regulatory elements found in non–coding regions of mRNAs. By binding small ligands riboswitches control gene expression in metabolic pathways of pathogenic bacteria. Therefore, they provide a promising target for antibacterial compounds.

The N1 synthetic riboswitch binds aminoglycoside antibiotics from the neomycin family. This riboswitch was shown to have regulatory activity in yeast (Duchardt–Ferner et al., *Angew. Chem. Int. Ed.* 2010, 49: 6216–6219). Structurally, it resembles the A–site, which is the well-known site in bacterial ribosomal RNA that binds aminoglycosides.

The aim of the project is to understand the ligand recognition mode of this aminoglycoside sensing riboswitch and the structural basis of its riboswitch activity. We performed all-atom molecular dynamics simulations of two different folds of the N1 riboswitch in the free and ligand–bound states. We investigated riboswitch complexes with two ligands: neomycin and ribostamycin, although the NMR structural data are available only for the complex with ribostamycin. We proposed the structure and equilibrium dynamics of the aminoglycoside-free riboswitch, which is unknown from experimental data. The observed conformational changes were compared with the NMR data and molecular dynamics simulations of the model of the ribosomal A–site. In the future we plan to enhance the sampling of conformational landscape of this riboswitch and perform replica exchange molecular dynamics .

26P

Deep moist atmospheric convection in a sub-kilometer global simulation

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(Yoshiaki Miyamoto, ymiyamoto@riken.jp)

A number of deep-moist convection exist on the earth at every moment. Temporal and spatial scales of the convection are 30 min – 1 hour and 1 – 10 km, respectively (e.g., *Byers and Braham 1948, Malkus 1952*). The convection plays an essential role in transporting energy in the troposphere and in determining the atmospheric structure. It has been impractical to simultaneously simulate all-scale phenomena from the convection (10^0 km) to global circulation (10^4 km) in a model due to their scale gap. Classically, the convection has been parameterized in atmospheric models in which the horizontal resolution ranged on the order of 10^1 to 10^2 km (e.g., *Arakawa and Schubert 1974*). Previous studies showed that the cloudy atmospheric disturbances are well simulated by such a global model (*Miura et al. 2007, Sato et al. 2009, Fudeyasu et al. 2010, Nasuno 2011*), though their grid spacings (several kilometers) were coarser than or comparable to the observed convection scale. With one of the fastest supercomputers, we first succeeded in conducting a global simulation with a sub-kilometer grid mesh that is finer than the convection scale. We here elucidate the convection features in the sub-kilometer simulation.

We utilized Nonhydrostatic ICosahedral Atmpospheric Model (NICAM, *Tomita and Satoh 2004*). The number of vertical layers was 94 and the grid interval gradually expanded with height. The physical processes such as solar radiation and boundary-layer turbulence were solved by the parameterizations. No cumulus parameterizations were used. The simulation periods were 12 hours. For specific details of experimental settings, see *Miyamoto et al. (2013).*
The global cloud distributions are well simulated: cloud clusters in the tropics, two tropical cyclones in the northwestern Pacific, mid-latitudinal disturbances and so on. In short, the sub-kilometer simulation successfully resolved multi-scale cloudy convective phenomena ranging from 10^0 to 10^4 km in a single simulation

27P

An Impact of Vertical Grid Arrangement in Baroclinic Wave Test

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RIKEN Advanced Institute for Computational Science

Baroclinic Wave Test is useful to assess a fundamental performance of dynamical core, and Jablonowski and Williamson (2006; JW06) is often used for this purpose. A vertical coordinate of the initial condition is based on pressure, and iteration process is needed to apply it to a model of height based vertical coordinate. However, the initial condition did not achieve a steady state on MPAS (Skamarock et al. 2012). For baroclinic wave, atmospheric conditions at lower troposphere would have large impact to simulated structures because variation of temperature and pressure are larger at lower level. Therefore, vertical resolution at lower level would be critical to achieve a steady state.

We tested an impact of vertical grid arrangement in the JW06 test case using three models, NICAM (Tomita et al. 2004, Satoh et al. 2008), MPAS (Skamarock et al. 2012), and ICON model (Wan et al. 2013). Tested horizontal grid spaces in ICON model are 158 km, 79 km, and 39 km. In NICAM and MPAS, horizontal grid spaces are 223 km, 112 km, and 56 km. Linear vertical arrangement (LVA) and stretched vertical arrangement (SVA) are tested with 40 and 80 levels. A thickness of LVA is 1125 m (constant), and the finest thickness is 58 m in SVA (40 levels, top-height=45,000 m).

Surface pressure distributions simulated by NICAM are shown in Figure 1, and wave patterns seems reasonable expect for cases with 40 levels with LVA. ICON model and MPAS also simulated a reasonable wave pattern and its development. To investigate difference of error amount among different vertical arrangements, we checked L2norm of surface pressure calculated using a numerical solution in highest horizontal grid-space for each models as a reference solution. ICON model showed reasonable convergence of a numerical solution with changing horizontal grid-space in any vertical arrangements. NICAM and MPAS with SVA showed reasonable convergence of numerical solutions changing horizontal grid-space. Although an improvement of error in numerical solution is found by refinement of horizontal grid space, an amount of improvement by vertical grid refinement is larger than that of horizontal improvement. It suggests that the important care is not only horizontal grid-space but also vertical grid-space to achieve higher resolution simulation. In the presentation, computational aspects also will be discussed.

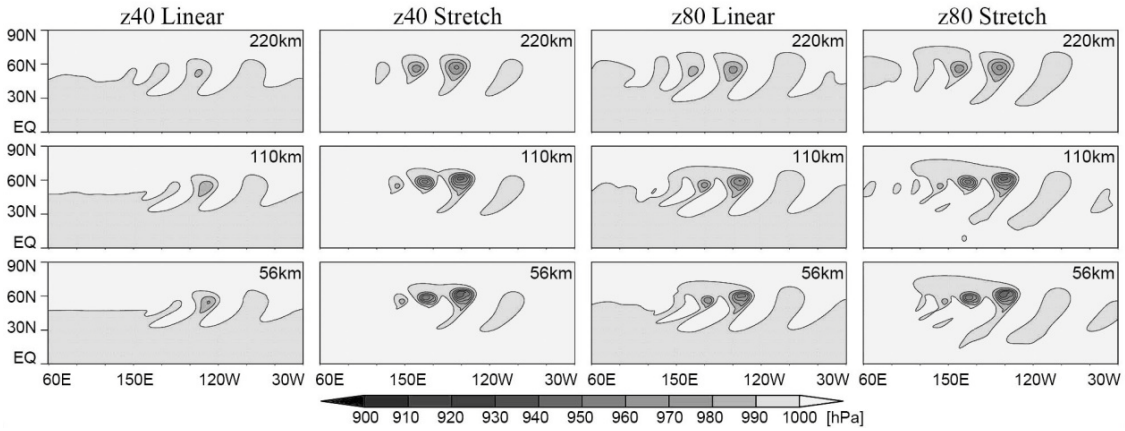

Figure 1: Surface Pressure distribution of NICAM in various horizontal and vertical resolutions. All panels shows fields after 9 days time-integration

28P

Impact of urban parameters in an urban canopy scheme on urban climate simulation

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[2]*Japan Agency for Marine-Earth Science and Technology, Japan*

More than half of people in the world live in urban areas. There is growing interest in an urban scheme in terms of adaptation study to future global warming as well as heat island research. The performance of urban climate simulation would depend on mainly two factors. One is the way of parameterization of urban morphology, the other is urban parameters given into an urban scheme. Regarding the former, the model performance was discussed in Grimmond et al. (2010) using 33 urban models from the point of view of energy balance between urban canopy and atmosphere. Thus, this study deals with the latter factor. The thermodynamic feature of a targeted urban area is expressed by changing urban parameters in a model, such as urban coverage ratio, sky view factor, heat capacity, thermal conductivity, albedo, roughness length, and so on. Recently, several studies put great effort to create the spatially-detailed database of urban information, although urban parameters are often assumed to be spatially homogeneous in the model. This study investigates the impact of spatially-detailed urban parameters on the performance of urban climate simulation.

The impacts of the gridded data of the urban fraction, the anthropogenic heat, and roughness length on summertime surface air temperature and surface wind speed are investigated by sensitivity experiment using WRF model. Surface air temperature is strongly affected by the land use. The difference of about 20% in urban fraction corresponds to the difference of about 0.6˚C in surface air temperature. The temperature difference between homogeneous AH run and gridded AH run is larger than 0.2˚C. The modified WRF represent the weakness of sea breeze as a result of large roughness length around Tokyo. The difference of surface wind speed is large in early evening because of the difference in decline speed of the mixing layer between urban and other land use areas.

29P

Conformational changes of SERCA in response to reactions described by hierarchical domain-motion analysis.

Chigusa Kobayashi[1], Ryotaro Koike[2], Motonori Ota[2], and Yuji Sugita[1,3,4,5]

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Sarco(endo)plasmic reticulum Ca^{2+}-ATPase (SERCA) pumps Ca^{2+} across membranes against a large concentration gradient. X-ray structures of the protein reveal rearrangement of transmembrane helices coupled with large-scale cytoplasmic domain motions. To characterize the conformational changes, we illustrate 'Motion Tree (MT)' based on crystal structures of SERCA. MT elucidates coupling between the motions of transmembrane helices and the cytoplasmic domain motions in individual reaction step. By gathering information from all MTs, rigid structural units of SERCA throughout the whole enzymatic cycle are identified. We discuss conformational changes of SERCA in response to individual reactions by characterizing its intrinsic conformational rigidity and flexibility.

30P

Local Ensemble Transform Kalman Filter Experiments with the Nonhydrostatic Icosahedral Atmospheric Model NICAM

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2: Atmosphere and Ocean Research Institute, The University of Tokyo, Kashiwa, Japan

The Local Ensemble Transform Kalman Filter (LETKF) is implemented with the Non-hydrostatic Icosahedral Atmospheric Model (NICAM) to assimilate the real-world observation data. First, the NICAM-LETKF system was developed using grid conversions between the NICAM's icosahedral grid and LETKF's longitude-latitude grid to take advantage of the existing codes. The grid conversions require additional computations and may cause additional interpolation error. Therefore, the LETKF code is modified, so that the LETKF reads and writes the NICAM's icosahedral grid data directly. We call this new version ICO-LETKF. In this study, the two systems are tested and compared using real conventional observations. The results show that the ICO-LETKF successfully accelerates the computations and improves the analyses.

31P

ParaHaplo: A program package for haplotype-based whole-genome association study on k computer.

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[1]Advanced Center for Computing and Communication, Riken, [2]StaGen Co., Ltd.

Background: More than a million single-nucleotide polymorphisms (SNPs) are analyzed in any given genome-wide association study (GWAS), therefore performing multiple comparisons can be problematic. One attempt to cope with multiple-comparison problems in GWAS was the development of haplotype-based algorithms to correct for multiple comparisons at multiple SNP loci in linkage disequilibrium (Misawa et al. 2008, J. Hum. Genet 53: 789-). In addition, permutation tests were found to also control problems inherent in multiple testing (Kimmel and Shamir 2006 Am. J. Hum. Genet. 79: 481-). However, both the calculation of exact probability and the execution of permutation tests are time-consuming and faster methods are required.

Methods: We developed a suite of computer programs, ParaHaplo. ParaHaplo can conduct parallel computation of accurate P-values in haplotype-based GWAS through use both Misawa et al.'s (2008) algorithm and Kimmel and Shamir (2006) algorithm. Our program is intended for workstation clusters and supercomputers using the Intel Message Passing Interface (MPI).

Results: We compared the performance of ParaHaplo on the HapMap dataset for Japanese in Tokyo, Japan and Han Chinese in Beijing, and Chinese. Computation was conducted on k computer.

Conclusion: The parallel version of ParaHaplo conducts genotype imputation much faster than the non-parallel version of ParaHaplo. ParaHaplo executable binaries and source code are available at
http://en.sourceforge.jp/projects/parallelgwas/releases/.

32P

Stability Analysis of Liquefaction Considering Soil-Water Coupling

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Advance Institute for Computational Science, RIKEN

Liquefaction refers to a sudden change in ground behavior from solid-like to fluid-like due to ground shaking. Despite the progresses made in previous experimental and numerical studies on liquefaction, the mathematical stability of the coupling of soil and water remains unclear. The mathematical stability refers to the existence of unstable solutions of the governing equations for the coupling of soil and water. Applying perturbation analysis, we seek to study the stability theoretically and numerically. Through the theoretical analysis of small perturbations in form of plane wave, we showed that the stability is lost when the degree of dilatancy exceeds a critical value. The numerical simulation of perturbations in form of spherical wave confirmed further the existence of unstable solution. Instability of the governing equations as shown in this paper calls for more cautious numerical treatment of liquefaction in future studies.

33P

Coarse-Grained model simulation of amyloid precursor protein in a mixed lipid membrane system

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The bio-membrane often forms nano-domains, rafts, and provides a special environment to a membrane protein. Amyloid precursor protein (APP) produces an Amyloid beta peptide, which is the source of senile plaque in a brain. The APP forms dimer or monomer conformations in the bio-membrane. Recent experiments have suggested that the cholesterols attach to the Gly-xxx-Gly motif, which is the interface motif of APP dimer conformation. We performed Martini Coarse-Grained (CG) model simulations of the APP and WALP23, which is a model membrane protein, with a mixed lipid membrane system, to understand the interaction between the proteins and lipids. We'll show the dynamics of these proteins in the mixed lipid bilayer environments.

34P

Kinetic Monte Carlo algorithm for thermally induced breakdown of fiber bundles

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Fiber bundle models are one of the most fundamental modelling approaches for the investigation of the fracture of heterogeneous materials being able to capture a broad spectrum of damage mechanisms, loading conditions, and types of load sharing. In the framework of the fiber bundle model we introduce a kinetic Monte Carlo algorithm to investigate the thermally induced creep rupture of materials occurring under a constant external load. We demonstrate that the method overcomes several limitations of previous techniques and provides an efficient numerical framework at any load and temperature values. We show for both equal and localized load sharing that the computational time does not depend on the temperature, it is solely determined by the external load and the system size. In the limit of low load where the lifetime of the system diverges, the computational time saturates to a constant value. Using this method we also check the Arrhenius law of lifetime for equal load sharing in the presence of any types of quenched disorder distributions. For localized load sharing, we show the modified form of the Arrhenius law does hold even in the presence of quenched disorder.

35P

Numerical Investigation for Electromagnetic Wave Propagation Phenomena using 3D Meshless Time Domain Method

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It is widely known that the finite difference time domain method (FDTDM) is applied to numerical analysis of electromagnetic wave propagation phenomena. In FDTDM, governing equations are discretized using the leap-frog method and the central difference method. Orthogonal meshes also known as staggered meshes must be applied to discretize governing equations. Therefore, Various devices are necessary for numerical analysis in complex shaped domain.

On the other hand, recently, the meshless method is applied to FDTDM. This method is called the meshless time domain method (MTDM). In MTDM, governing equations are discretized using the leap-frog method, shape functions and partial derivatives of the shape functions. Orthogonal meshes do not need to be applied to discretize governing equations. Therefore, numerical analysis in complex shaped domain is executed easily. However, in the previous study, the influence of the weight function on computational precision or numerical stability is not clear in three-dimensional MTDM.

The purpose of this study is to investigate effects of the weight function on the computational precision and the numerical stability of 3-D MTDM.

36P

Traffic Simulation of Kobe-city

Yuta Asano [A], Nobuyasu Ito [A, B, C], Hajime Inaoka [A, C],
Yohsuke Murase [A, C], Tetsuo Imai [A, C], Takeshi Uchitane [A, C]
[A] *RIKEN, AICS* [B] *Dept. of App. Phys., The Univ. of Tokyo* [C] *CREST, JST*

Cars and trains play major roles in today's urban mobility. It is not too much to say that people is living in automobile-dependent community. On the other hand, social problems such as a traffic jam are becoming a remarkable matter. The traffic jam poses disadvantage to daily life and economics. In addition, it also affects global warming and other environmental problems.

A traffic simulation becomes a way to resolve these problems, because today's computer has the ability to execute large scale simulation in a practical time. In this study, a traffic simulation of Kobe-city is carried out to resolve the social problems. Almost all these kind of simulations have used the OpenStreetMap (OSM) [1] for convenience. However, in the sense that the purpose of the simulation is to the resolve actual traffic problems, the OSM is not necessary sufficient, because there are difference from an actual road structure. Therefore, the road structure was built utilizing a high-quality digital map data constructed by Zenrin Co. Ltd.

Although various traffic simulators exist, SUMO (Simulation of Urban Mobility) [2] was adopted. A method of the traffic simulation utilizing SUMO consists of building the road structure and estimating an origin-destination (OD) information. The OD information was estimated by a geographical population distribution estimated by NTT DoCoMo, Inc. from its mobile phone position data.

The amount of traffic flows obtained from the simulation were deviated from that of the traffic census data [3]. We expect that a routing algorithm of SUMO and the OD information is unrealistic. Therefore, to conduct the traffic simulation of Kobe-city, it is necessary to improve the routing algorithm and the OD information.

[1] http://www.openstreetmap.org/
[2] D. Krajzwics, et al., International Journal On Advances in Systems and Measurements 5 (2012) 128.
[3] http://www.city.kobe.lg.jp/information/data/statistics/traffic/keikaku/traffic.html

37P

Toward investigating the impacts of dense and frequent surface observations on severe rainstorm forecasts

Yasumitsu Maejima[1], Masaru Kunii[2], Hiromu Seko[2],
Ryota Maeda[3], Kae Sato[3] and Takemasa Miyoshi[1]

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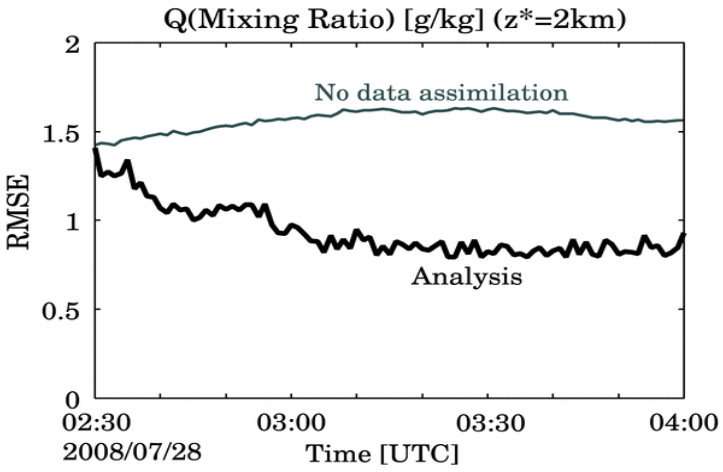
2. Meteorological Research Institute, Japan Meteorological Agency, Japan
3. Meisei Electric Co., Ltd, Japan

To investigate the impacts of observations with high spatial and temporal density on local heavy rainfall prediction, we performed a numerical simulation at a 100-m resolution and a series of Observing System Simulation Experiments (OSSEs) using the Local Ensemble Transform Kalman Filter (LETKF) with the JMA-NHM (NHM-LETKF) at a 1-km resolution.
First, we performed a numerical simulation using the JMA-NHM downscaled from 5 km to 100 m horizontal resolutions. This simulation is used as the nature run for the OSSEs. The nature run contains a precipitation band with its maximal intensity > 100 mm/h. The associated cold pool and divergent flow at the lower troposphere contribute to the sustained development of the precipitation band.

Next, we simulated a synthetic radar observations every 1 minute from the nature run, and performed a data assimilation experiment using the NHM-LETKF system. The figure shows a time series of the root mean square errors (RMSE) of water vapor and other hydrometeors. When the radar data are assimilated (thick curve), the RMSE became much lower than the case without radar data (thin curve).

We will investigate the impact of additional ground observations to discuss effective surface observing strategy such as locations and frequency of observations.



38P

A mosaic of water orientation structures at a neutral zwitterion lipid/water interface revealed by molecular dynamics simulations

Suyong Re,[†] Wataru Nishima,[†,¶] Tahei Tahara,[‡,§] and Yuji Sugita*[,†,#,$,¶]

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Ordering of water structures near the surface of biological membranes has been recently extensively studied using interface-selective techniques like vibrational sum-frequency generation (VSFG) spectroscopy. The detailed structures of interface water have emerged for charged lipids, but those for neutral zwitterionic lipids remain obscure. We analyze an all-atom molecular dynamics (MD) trajectory of hydrated 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine bilayer to characterize the orientation of interface waters in different chemical environments. Structure and dynamics of interfacial waters strongly depend on both their vertical position along the bilayer normal as well as vicinal lipid charged groups. Water orientation in the vicinity of phosphate groups is opposite to that around choline groups. The results are consistent with observed VSFG spectra and demonstrate that a mosaic of water orientation structures exists on the surface of a neutral zwitterionic phospholipid bilayer reflecting rapid water exchange and influence of local chemical environments.

39P

Transition from cumulus under stratocumulus to isolated cumulus simulated in a single calculation domain

Yousuke Sato
Advanced Institute for Computational Science, RIKEN

The transition from high cloud cover to low cloud cover of stratocumulus was well simulated in a single calculation domain of a large eddy simulation model with fine grid resolution (Δx=50m) covering wide calculation domain (300 km x 30 km). The results indicated that shallow cloud cover is controlled by two important factors, the horizontal convection distance and cloud broadening distance at the top of the boundary layer.

High cloud cover with “cumulus under stratocumulus” occurs when there is large cloud broadening at the boundary layer top and a short convection distance. In contrast, low cloud cover with “isolated cumulus” occurs when there is a small broadening and a long convection distance. It is also found from the result that surface flux rather than the amount of aerosol has primary effects on the broadening distance.

40P

Fault and failure analysis on the K computer

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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 is more than 1,000,000. The ratio of irregular system down time is no more than 1.6% as shown in Fig1.

The stability of the K computer is primarily contributed by the system design of the K computer. We took reliability, availability and serviceability into account for K computer's design concept because K computer consists of huge number of parts. In order to reduce system faults and failures K computer adopted some new functions.

In this poster, we introduce the design concept for reliability, availability and serviceability of the K computer and the implementation. Then we analyze trends of faults and failures on the K computer for two years and consider way to reduce service down time.

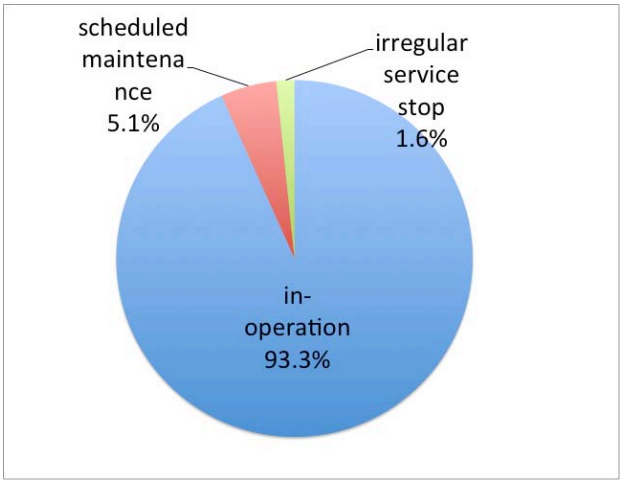

Fig1. Operation time of the K computer since Sep. 2012.

41P

Kobe city's translocation-agent-based epidemic model simulation

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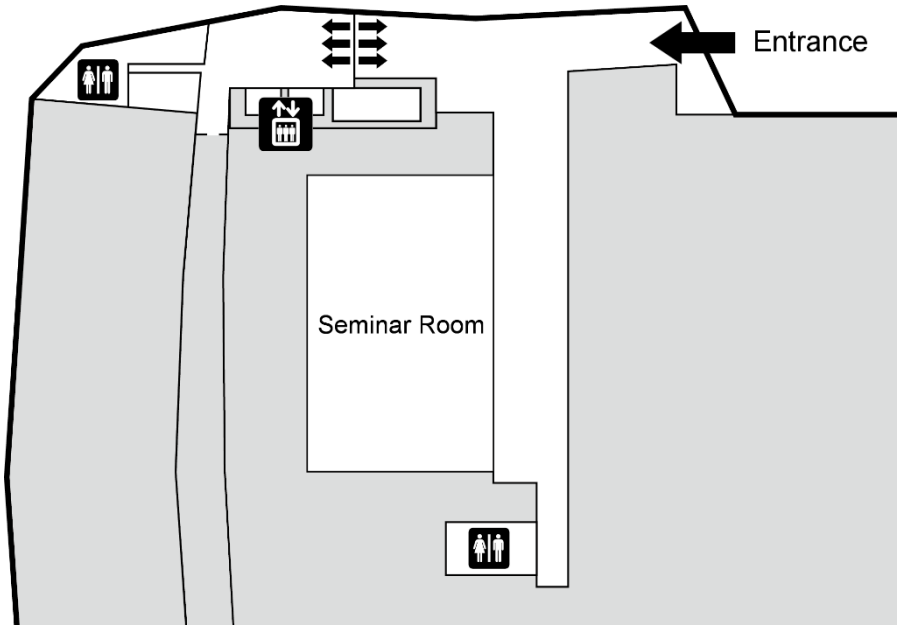
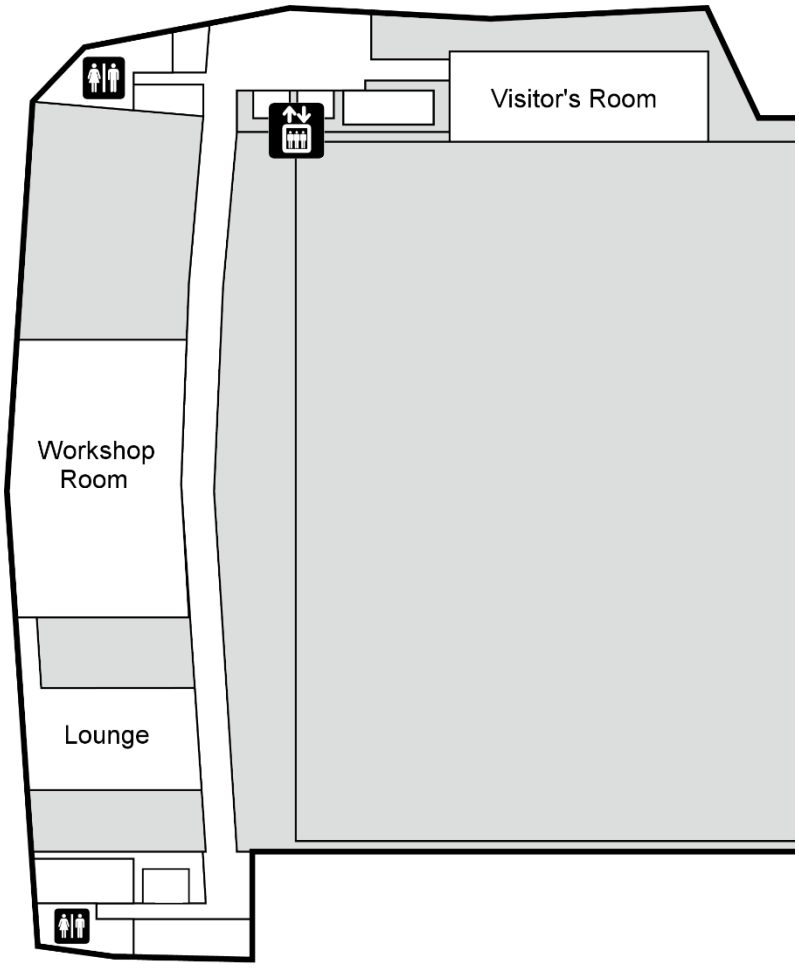
The first part of this post present a agent-based epidemic model for studying how the population's density, social interacting and movement speed up the epidemic propagating. In this model, the researchers can set epidemic and immunization parameters, such as how many days of recovering and the difficulty of been infected of each agent. Our result shows agents in two-dimensional square and hexagon social interacting networks that population of infected S(t) increases as time $S(t) \sim t^2$, instead of Susceptible-Infected-Recovered (SIR) model's exponential increasing $S(t) \sim exp(\beta t)$. A population density threshold ρ_c that will not rising a global infection, $\rho < \rho_c$ $S(\infty)=0+$,is found in our model and the threshold value will increase while agents move. The second part shows the epidemic simulation of the downtown area of Kobe city's according to the population.

Floor Map

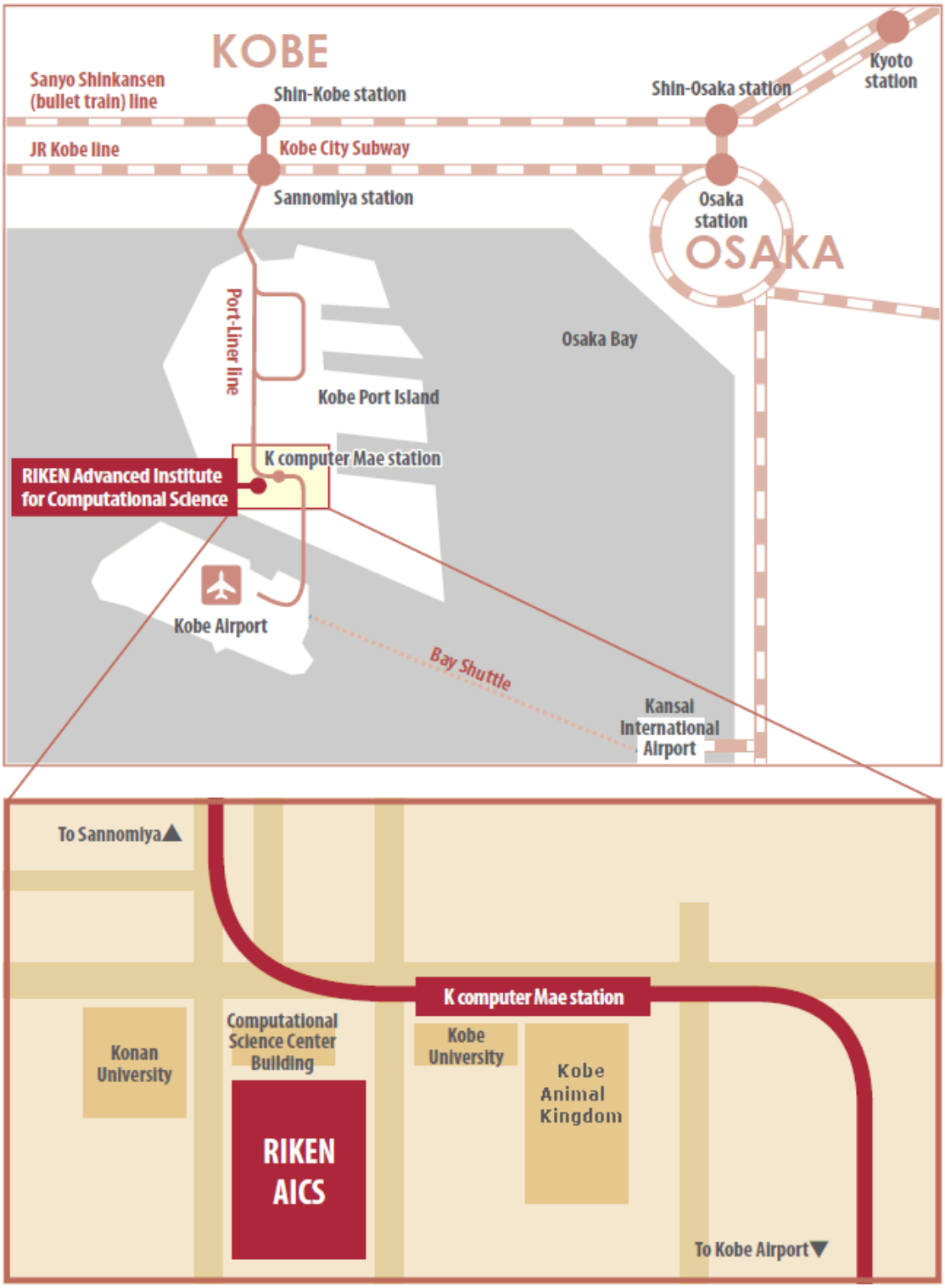
1st floor



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
K computer Mae station
RIKEN Advanced Institute for Computational Science
Kobe Airport
Bay Shuttle
Kansai International Airport
To Sannomiya▲
K computer Mae station
Konan University
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