Review of the Center for Computational Sciences University of Tsukuba 2020

筑波大学 計算科学研究センター 外部評価報告書

筑波大学

University of Tsukuba

2020

Review of the Center for Computational Sciences University of Tsukuba

筑波大学 計算科学研究センター 外部評価報告書

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筑波大学計算科学研究センター 外部評価報告書

September 2020

2020 年 9 月

Center for Computational Sciences

University of Tsukuba

Foreword

This volume contains the Report of the External Review for Center for Computational Scineces (CCS), University of Tsukuba, which was carried out in FY2019. The objective of the External Review was to evaluate the research activities of CCS during the period from FY2014 to FY2019 since the previous external review which was held in FY2013, and the future strategy and plans.

Originally formed as the Center for Computational Physics (CCP) in 1992, the CCS was reorganized, expanded and relaunched under its current name in April 2004. The mission of the Center for Computational Sciences (CCS) is the promotion of "Multidisciplinary Computational Sciences" through enhanced cooperation between, and the fusion of, computational and computer sciences. The most important characteristics of the research collaboration in the CCS is “codesigning” where the needs from application fields and seeds from system technologies to make a balanced and optimized system development as well as application program development. As a unique research center where both computational and computer scientists work together, our codesigning for advanced High Performance Computing (HPC) research has been continued from the beginning until today.

The CCS has developed several supercomputers, and conducted computational sciences in the areas of particle physics, astrophysics, nuclear physics, materials science, life science, environmental science, high performance computing technology, and information science including database technology and computational media. Also, the CCS plays a significant role as a nation-wide joint-use facility that provides computational resources for external scientific researchers in all of these areas all over the world. Since 2010, the CCS has been approved as a “national core-center” under the Advanced Interdisciplinary Computational Science Collaboration Initiative (AISCI) launched by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan. After High Performance Computing Infrastructure (HPCI) project started under MEXT on 2012, the supercomputers at CCS have been partially contributed to this nation-wide resource sharing program.

Before the External Review, we prepared the documents of Summary of Activities (Part I), Activities, Results and Collaborations in the research divisions and public relations (Part II), and Strategy and Future Plans (Part III), all of which are contained in this volume. The review was carried out on February 19th to 21st in 2020, where the all the activities in CCS was reported and a lot of discussion was made. The external review committee was composed of 11 members who were Prof. William Gropp (chair, National Center for Supercomputing Applications, USA), Prof. Masaki Sato (vice chair, the University of Tokyo, Japan), Prof. Chris Sachrajda (University of Southampton, UK), Prof. Lars Hernquist (Harvard University, USA), Prof. Pieter Maris (Iowa State University, USA), Prof. Angel Rubio (Max Planck Institute for Structure and Dynamics Matter, Germany and Flatiron Institute, USA), Prof. John Zhang (New York University Shanghai, China), Prof. Shiguang Miao (China Meteorological Administration, China), Prof. Hiroshi Nakashima (Kyoto University, Japan), Prof. Jeffrey Xu Yu (Chinese University of Hong Kong, Hong Kong), and Prof. Bruce H. Thomas (the University of South Australia, Australia).

The external review committee reviewed the CCS activities very carefully, and in the report, endorsed the activities and future strategy and plans of the CCS. The report encourages us towards the further development of “Multidisciplinary Computational Sciences” in CCS. On behalf of CCS, I would like to thank most deeply all of the external review committee members for providing such a valuable report. Also, I specially appreciate a great cooperation by Prof. Gropp as chair and Prof. Sato as vice chair to summarize the report.

At the end of this forword, I must note that this review discussion with the external review committee had been carried out just before the world wide infectious disease by the new type coronavirus started at the end of 2019 (COVID-19). Just a couple of weeks after the review meeting, our life was totally changed including a strong restriction of transportation between countries which hugely impacted our research especially on world wide collaboration. Actually, one of the committee member could not join to in-person meeting at CCS due to regulation made by Japanese government for COVID-19, but we could make it through on-line interview and discussion with him. All other members could join, and we could carry out the review meeting completely on schedule. I think that we were merely lucky and am truly happy to complete this work. I hope all the health of people involved in this review work.

August 2nd, 2020

Taisuke Boku
Director of Center for Computational Sciences
University of Tsukuba

まえがき

この報告書は、2019 年度に行われた、筑波大学計算科学研究センター（以下 CCS）の外部評価の結果をまとめたものである。外部評価の目的は、2013 年度に行われた前回の外部評価以降の 2014 年度から 2019 年度までの活動、ならびに今後の戦略と計画について評価を受けることである。

計算科学研究センターは、1992 年（平成 4 年）度に設立された計算物理学研究センターを前身とし、2004 年（平成 16 年）4 月に改組・拡充により再設立された。CCS は、科学諸分野と計算機科学分野の協働･融合を軸とした「学際計算科学」を推進している。CCS における活動で最も特徴的なことは、応用分野のニーズと計算機システム技術のシーズの双方の観点からの議論により、問題解決のために最適化されたバランスのとれた計算機システムを開発するコデザイン（codesigning）に基づく研究を行っていることである。これは、科学諸分野の研究者と計算機システム研究者の双方が共存するという、我が国でも特別な CCS の研究環境だからこそなし得ることであり、CCS はその設立から今日に至るまでの研究を継続している。

CCS では、数々のスーパーコンピュータの開発を行うと共に、素粒子、宇宙、原子核、物質、生命、地球環境、高性能計算システム、データ基盤、計算メディア等の科学の諸領域における計算科学の研究を行っている。また、これらの計算科学研究に従事する国内及び海外の研究者に計算機資源を提供する、全国共同利用施設としての役割も担っており、2010 年（平成 22 年）には、文部科学省共同利用・共同研究拠点「先端学際計算科学共同研究拠点」（Advanced Interdisciplinary Computational Science Collaboration Initiative: ACSCI）に認定された。さらに、2012 年（平成 24 年）に文部科学省において「革新的ハイパフォーマンス・コンピューティング・インフラ」（High Performance

Computing Infrastructure: HPCI）が開始されて以来、CCS のスーパーコンピュータはその計算資源の一翼を担っている。

外部評価に先立ち、資料として 2014 年度から 2019 年度の活動全体（Part I）、各研究部門・研究分野及び広報室の活動実績（Part II）、今後の戦略と将来計画（Part III）を取りまとめた（本冊子に掲載）。外部評価は、2020 年 2 月 19 日〜21 日の 3 日間に行われ、センターの活動を報告し、これについて外部評価委員と多くの詳細な議論が行われた。評価委員会は、William Gropp 教授 (委員長, National Center for Supercomputing Applications, USA), 佐藤正樹教授 (副委員長, 東京大学), Chris Sachrajda 教授 (University of Southampton, UK), Lars Hernquist 教授 (Harvard University, USA), Pieter Maris 教授 (Iowa State University, USA), Angel Rubio 教授 (Max Planck Institute for the Structure and Dynamics of Matter, Germany and Flatiron Institute, USA), John Zhang 教授 (New York University Shanghai, China), Prof. Shiguang Miao 教授 (China Meteorological Administration, China), 中島浩教授(京都大学), Jeffrey Xu Yu 教授 (Chinese University of Hong Kong, Hong Kong), Bruce H. Thomas 教授 (The University of South Australia, Australia)の計 11 名である。

外部評価委員は CCS における活動を注意深く評価し、本報告においてその活動と今後の戦略と計画について支持している。本報告は「学際計算科学」に関する CCS としての今後の研究活動を強く勇気づけてくれるものである。CCS を代表し、外部評価委員会の全ての委員に対し、このように価値ある報告書を作成頂いたことに感謝したい。特に、委員長の Gropp 教授と副委員長の佐藤教授には、報告書取りまとめ作業におけるご苦労に、特段の謝意を表したい。

この前書きの最後に、ぜひ特筆しておきたいことがある。本外部評価会議は、2019 年末に始まった世界規模の新型コロナウィルス感染症拡大（COVID-19）が深刻化する、まさに直前に行われた。会議のわずか数週間後には世界はこの歴史的大問題に直面し、国を跨いだ移動制限を始めとする様々な問題によって我々の生活は一変し、特に国際的な共同作業は大きな影響を受けることになった。事実、外部評価委員会のうち 1 名の委員は、日本国が定めた海外からの渡航制限により、CCS における委員会に直接参加することが不可能となったが、他の全委員は問題なく参加し、当該委員もオンライン形式で報告と議論に参加することができ、結果として会議は予定通り開催され滞りなく終了した。このことについて、我々はまさに幸運であったとしか言いようがない。本外部評価作業に携わった全ての方々の健康を祈り、前書きの結びとしたい。

2020 年 8 月 2 日
筑波大学　計算科学研究センター
センター長　朴泰祐

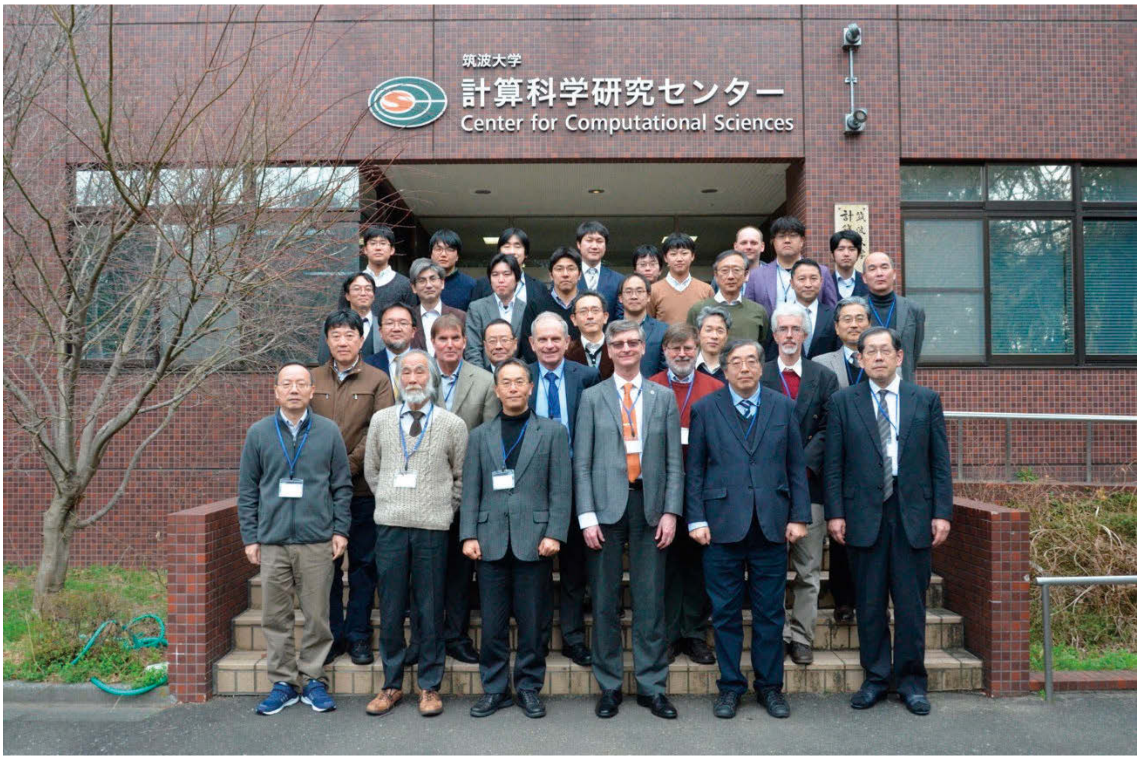
Member List of the External Review Committee

外部評価委員会委員リスト

Name	Research Field	Title, Affiliation
William Gropp (Chair)	Computer Science 計算機科学	Director National Center for Supercomputing Applications, USA
Masaki Sato (Vice Chair)	Environmental Science 地球科学	Professor Atmosphere and Ocean Research Institute The University of Tokyo, Japan
Chris Sachrajda	Particle Physics 素粒子物理学	Professor Department of Physics and Astronomy University of Southampton, UK
Lars Hernquist	Astrophysics 宇宙物理学	Professor Harvard-Smithsonian Center for Astrophysics Harvard University, USA
Pieter Maris	Nuclear Physics 原子核物理学	Professor Iowa State University, USA
Angel Rubio	Material Science 物質科学	Director, Theory Department, Max Planck Institute for the Structure and Dynamics of Matter, Germany & Distinguish Research Scientist, Center for Computational Quantum Physics, Flatiron Institute, USA
John Zhang	Biological Science 生命科学	Professor NYU-ECNU Center for Computational Chemistry New York University Shanghai, China
Shiguang Miao	Geoscience 地球科学	Professor, Director Institute of Urban Meteorology China Meteorological Administration, China
Hiroshi Nakashima	Computer Science 計算機科学	Professor Academic Center for Computing and Media Studies Kyoto University, Japan

Jeffrey Xu Yu	Database / Informatics データベース/情報学	Professor Department of Systems Engineering and Engineering Management Chinese University of Hong Kong, Hong Kong
Bruce H. Thomas	Media Science / Informatics メディア科学/情報学	Professor School of Information Technology and Mathematical Sciences The University of South Australia, Australia

Photo of the External Review 2020



External Review Schedule 2020

February 2020

Center for Computational Sciences
University of Tsukuba

External Review on Center for Computational Sciences, University of Tsukuba

Date: February 19th, 20th and 21st, 2020
Place: Center for Computational Sciences, University of Tsukuba
(https://www.ccs.tsukuba.ac.jp)

External Review Committee:

William Gropp (Chair)	Computer Science, Director National Center for Supercomputing Applications, USA
Masaki Sato (Vice Chair)	Environmental Science,Professor Atmosphere and Ocean Research Institute The University of Tokyo, Japan
Chris Sachrajda	Particle Physics, Professor Department of Physics and Astronomy University of Southampton, UK
Lars Hernquist	Astrophysics, Professor Harvard-Smithsonian Center for Astrophysics Harvard University, USA
Pieter Maris	Nuclear Physics, Professor Iowa State University, USA
Angel Rubio	Material Science, Director, Theory Department, Max Planck Institute for Structure and Dynamics of Matter, Germany & Distinguish Research Scientist, Center for Computational Quantum Physics, Flatiron Institute, USA
John Zhang	Biological Science, Professor NYU-ECNU Center for Computational Chemistry New York University Shanghai, China
Shiguang Miao	Geoscience, Director Institute of Urban Meteorology China Meteorological Administration, China
Hiroshi Nakashima	High Performance Computing, Professor Academic Center for Computing and Media Studies Kyoto University, Japan

Jeffrey Xu Yu	Database / Informatics, Professor Department of Systems Engineering and Engineering Management Chinese University of Hong Kong, Hong Kong
Bruce H. Thomas	Media Science / Informatics, Professor School of Information Technology and Mathematical Sciences The University of South Australia, Australia

Program

19th February (Wednesday)

Overview of CCS (**Workshop Room**)

10:00-11:00 Welcome & Overview of CCS (T. Boku, Director of CCS)

11:00-11:30 Activities and Results 2014-2018 (M. Umemura, ex-Director of CCS)

11:30-10:45 Coffee Break

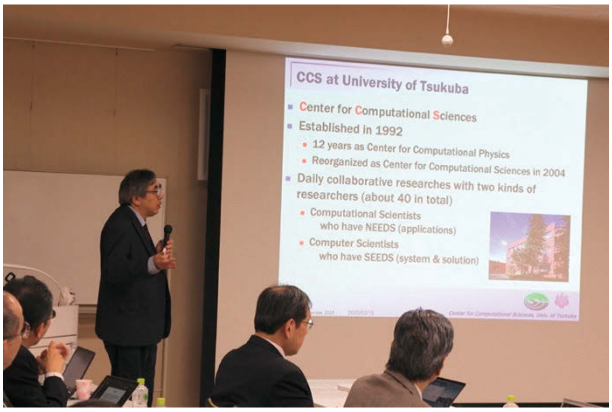
11:45-12:05 Supercomputer-I: Oakforest-PACS System (O. Tatebe, CCS)

12:05-12:25 Supercomputer-II: Cygnus System (T. Boku, Director of CCS)

12:25-12:45 ILDG/JLDG Project (T. Yoshie)

12:45-13:00 Visiting Cygnus Supercomputer

13:00-14:00 Lunch



T. Boku, Director of CCS

M. Umemura, ex-Director of CCS

O. Tatebe, Computer System Manager of CCS

T. Yoshie

T. Boku

Visiting Cygnus Supercomputer

Activities & Collaborations of Divisions (**Workshop Room)**

14:00-14:30 REPORT: Division of Particle Physics (Y. Kuramashi)

14:30-15:00 REPORT: Division of Astrophysics (M. Umemura)

15:00-15:30 REPORT: Division of Nuclear Physics (T. Nakatsukasa)

15:30-15:45 Coffee Break

15:50-16:20 REPORT: Division of Quantum Condensed Matter Physics (K. Yabana)

16:20-16:50 REPORT: Division of Life Sciences (Y. Shigeta & Y. Inagaki)

16:50-17:20 REPORT: Division of Global Environmental Science (H. Kusaka)

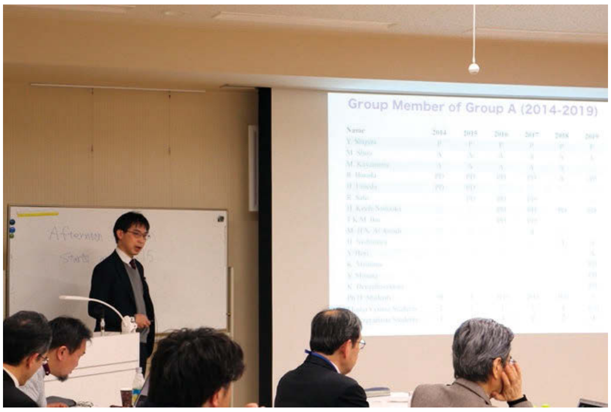
17:20-17:30 Wrapping up DAY1

17:30-18:30 Reception

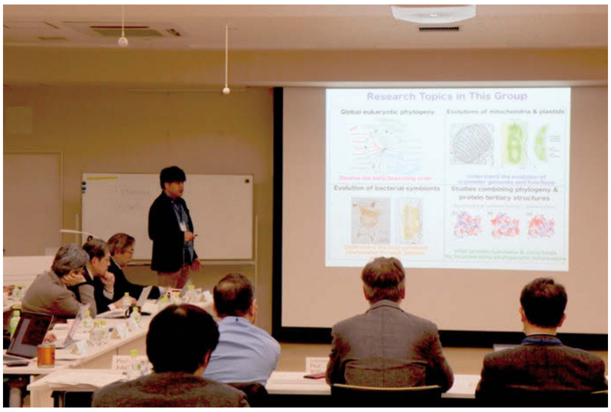
Y. Kuramashi

K. Yabana

T. Nakatsukasa



Y. Shigeta



Y. Inagaki

H. Kusaka

20th February (Thursday)

Activities of Divisions (cont'd) (**Workshop Room)**

9:30-10:00 REPORT: Division of High Performance Computing Systems (T. Boku)

10:00-10:30 REPORT: Division of Computational Informatics: Database Group (H. Kitagawa)

10:30-11:00 REPORT: Division of Computational Informatics: Computational Media Group (Y. Kameda)

11:00-11:20 Coffee Break

11:20-11:35 Project Office for Exascale Computational Sciences (K. Yabana)

11:35-11:50 Project Office for Exascale Computing System Development (T. Boku)

11:50-12:05 Department of Computational Medical Science (M. Umemura)

12:05-12:35 Project Office for AI & Big Data (T. Amagasa)

12:35-14:00 Project Office for HPCI (Y. Kuramashi)

12:35-14:00 Lunch

H. Kitagawa

Y. Kameda

T. Amagasa

M. Umemura

Breakout Sessions

14:00-18:30

Division of Particle Physics Reviewer: Chris Sachrajda	Room: SB-1112
Division of Astrophsyics Reviewer: Lars Hernquist	Room: CCS-Workshop
Division of Nuclear Physics Reviewer: Pieter Maris	Room: SB-911-1
Division of Quantum Condensed Matter Physics Reviewer: Angel Rubio	Room: CCS-C
Division of Life Sciences Reviewer: John Zhang	Room: SB-1001
Division of Global Environmental Science Reviewer: Masaki Sato, Shiguang Miao	Room: CCS-B
Division of High Performance Computing Systems Reviewer: Hiroshi Nakashima, William Gropp	Room: CCS-A
Division of Computational Informatics: Database Group Reviewer: Jeffrey Xu Yu	Room: SB-911-2
Division of Computational Informatics: Computational Media Group Reviewer: Bruce H. Thomas	Room: SB-1111

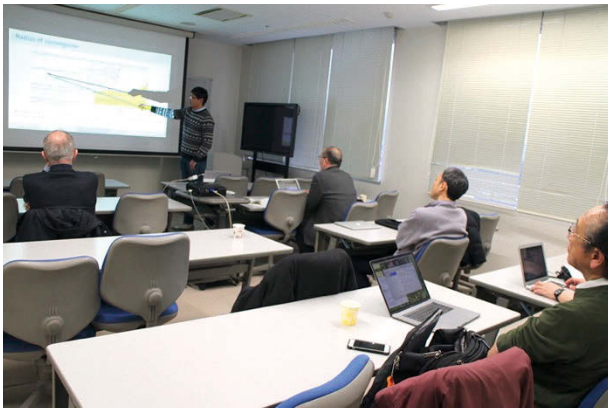
18:30-19:00 Closing of DAY2 & Moving to Dinner Restaurant

19:00-21:00 Committee Dinner Meeting

Breakout Sessions: Division of Particle Physics

Reviewer: Chris Sachrajda Room:SB-1112

START	END	SPEAKER	TOPIC
14:00	14:10	Y. Kuramashi	Overview
14:10	14:30	Y. Kuramashi	Master field simulation in 2+1 flavor QCD
14:30	14:55	T. Yamazaki	Hadron form factors
14:55	15:20	N. Ishizuka	K→ππdecay amplitude with Wilson-type quarks
15:20	15:40		COFFEE BREAK
15:40	16:05	K.Kanaya	QCD thermodynamics with gradient flow
16:05	16:30	H. Ohno	QCD at non-zero temperature and density with Highly Improved Staggered Quarks
16:30	16:50	Y. Kuramashi	Determination of critical end point in 3 flavor QCD
16:50	17:10		COFFEE BREAK
17:10	17:35	T. Yoshie	Numerical study of CFTs
17:35	18:00	Y. Kuramashi	Application of TN scheme to QFTs



H. Ohno (Particle Physics)

Breakout Sessions: Division of Astrophysics

Reviewer: Lars Hernquist Room: CCS-Workshop

START	END	SPEAKER	TOPIC
14:00	14:15	K. Yoshikawa	Neutrinos & LSS
14:15	14:30	H. Yajima	Galaxy formation
14:30	14:45	A. Wagner	AGN feedback
14:45	15:00	M. Umemura	BH merger & SMBH
15:00	15:15	M. Mori	Galactic archeology
15:15	15:30	K. Ohsuga	BH accretion & outflows
15:30	15:45	K. Furuya	Protoplanetary chemistry
15:45	16:00	Y. Takamizu	Early Universe
16:00	16:30		COFFEE BREAK
16:30	16:45	S. Inoue	Galactic structure
16:45	17:00	M. Abe	SEURAT
17:00	17:15	K. Yoshikawa	Radiative transfer on GPU/FPGA
17:15	17:30	K. Ohsuga	GRRMHD
17:30	17:45	M. Umemura	Turbulent clustering of dust
17:45	18:00	H. Fukushima	Circlularly polarized light generation
18:00	18:15	H. Yajima	Bioimaging - TRINITY


K. Ohsuga (Astrophysics)


K. Furuya (Astrophysics)

Breakout Sessions: Division of Nuclear Physics

Reviewer: Pieter Maris Room: SB-911-1

START	END	SPEAKER	TOPIC
14:00	14:10	B. Kumar	Probe the EoS with dark matter and neutron stars
14:10	14:40	T. Nakatsukasa	Structure of neutron-star inner crust and pulsar glitches
14:40	15:10	N. Hinohara	Recent development of finite-amplitude method for nuclear density functional theory
15:10	15:25		COFFEE BREAK
15:25	16:05	Y. Hashimoto	Fusion/fission with Gogny-TDHFB/CbTDHFB
16:05	16:35	K. Wen	Adiabatic self-consistent collective reaction path for nuclear reactions
16:35	17:00	T. Nakatsukasa	Requantization of TDHFB alternative to GCM
17:00	17:15		COFFEE BREAK
17:15	17:45	N. Hinohara	Calculation of neutrinoless double-beta decay nuclear matrix elements and role of isoscalar neutron-proton pairing
17:45	18:10	T. Nakatsukasa	ImPACT Project: Reduction and resource recycling of high-level radioactive wastes through nuclear transmutation
18:10	18:30		Discussion

Y. Hashimoto (Nuclear Physics)

Breakout Sessions: Division of Quantum Condensed Matter Physics

Reviewer: Angel Rubio Room: CCS-C

START	END	SPEAKER	TOPIC
14:00	14:10	K. Yabana	Introduction
14:10	14:40	H. Koizumi	Strongly correlated systems
14:40	15:10	X.-M. Tong	Atomic physics
15:10	15:40	N. Maeshima	Optical response of solids
15:40	16:00		COFFEE BREAK
16:00	16:20	A. Hashmi	Two-dimensional materials
16:20	16:40	A. Yamada	Light-induced molecular dynamics
16:40	17:00	M. Noda	Large-scale calculation for nano-optics
17:00	17:20	T. Takeuchi	Optical response of meta-surface
17:20	17:40	S. Yamada	Optical response of thin films
17:40	18:00		Discussion

X.-M. Tong (Quantum Condensed Matter Physics)

Breakout Sessions: Division of Life Sciences

Reviewer: John Zhang Room: SB-1001

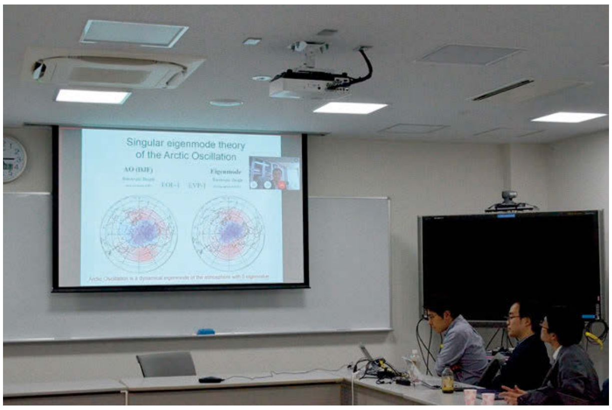
START	END	SPEAKER	TOPIC
14:00	14:25	Y. Inagaki	Molecular Evolution
14:25	14:50	Y. Isitani	Molecular Evolution
14:50	15:00		COFFEE BREAK
15:00	15:25	M. Shoji	Enzymatic reaction
15:25	15:50		Quantum Biology
15:50	16:00		COFFEE BREAK
16:00	16:25	R. Harada	Molecular Dynamics Simulation
16:25	16:40	H. Nishizawa	QM/MM simulation
16:40	16:50		COFFEE BREAK
16:50	17:05	Y. Hori	Proton conductance
17:05	17:30	Y. Shigeta	Photochemistry and Astrobiology
17:30	18:00		Discussion

Y. Hori (Biological function and information group)

Breakout Sessions: Division of Global Environmental Science

Reviewer: Masaki Sato, Shiguang Miao Room: CCS-B

START	END	SPEAKER	TOPIC
14:00	14:30	H. Kusaka	Research activity during the last five years by Kusaka Group
14:30	15:00	H. Tanaka (M. Matsueda)	Progress in general circulation study during the last five years by Tanaka Group
15:00	15:15		COFFEE BREAK
15:15	15:45	M. Matsueda	Research activities in FY 2015-2019 by Matsueda Group
15:45	16:15	A. Yamagami	Predictability in the Arctic cyclones
16:15	16:30		COFFEE BREAK
16:30	17:00	A. Nishi	Local winds study
17:00	17:30	D. Q. Van (H. Kusaka)	Urban climate study
17:30	17:45		COFFEE BREAK
17:45	18:00	All	Discussion



M. Matsueda (Global Environmental Science)

Breakout Sessions: Division of High Performance Computing Systems

Reviewer: Hiroshi Nakashima, William Gropp Room: CCS-A

START	END	SPEAKER	TOPIC
14:00	14:15	T. Boku	Supercomputer development in CCS
14:15	14:45	T. Boku	Collaboration with application fields
14:45	15:15	D. Takahashi	Numerical computation, FFT
15:15	15:35		COFFEE BREAK
15:35	16:05	O. Tatebe	File I/O and System Software
16:05	16:35	H. Tadano	Numerical computation, Krylov
16:35	17:05	R. Kobayashi	GPU/FPGA computing
17:05	17:25		COFFEE BREAK
17:25	17:55	N. Fujita	Parallel FPGA computing
17:55	18:25	Y. Yamaguchi	FPGA

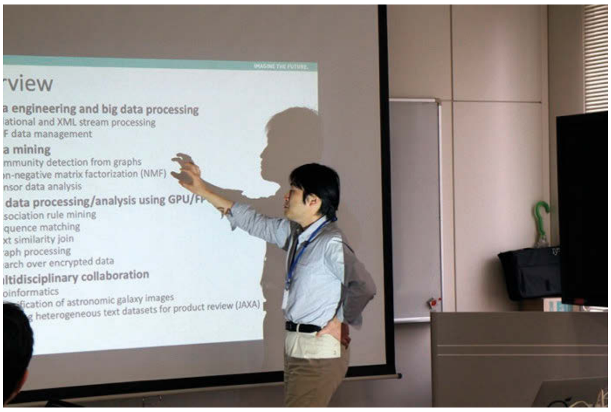
N. Fujita (HPC systems)

H. Tadano (HPC systems)

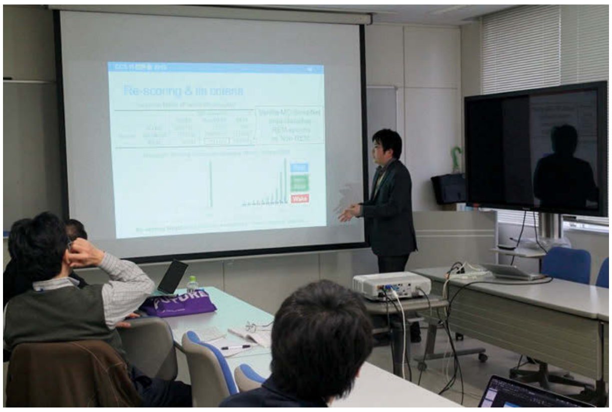
Breakout Sessions: Division of Computational Informatics: Database Group

Reviewer: Jeffrey Xu Yu Room: SB-911-2

START	END	SPEAKER	TOPIC
14:00	14:30	H. Kitagawa	Overview, Information Integration, Outlier, Social Media
14:30	15:00	T. Amagasa	Data Analysis using GPU/FPGA, XML, Open Data, Privacy
15:00	15:30	H. Shiokawa	Graph Data Analysis
15:30	15:45		COFFEE BREAK
15:45	16:15	K. Horie	Sleep Data Analysis, Noise Reduction
16:15	16:35	L. Ota	Sleep Data Analysis
16:35	16:55	R. Miyamoto	Sleep Data Analysis
16:55	17:10		COFFEE BREAK
17:10	17:30	H. Itoh	NMF and Community Detection
17:30	17:50	B. Happy	Knowledgebase Question Answering
17:50	18:30	H. Kitagawa	Discussion



T. Amagasa (Database Group)



K. Horie (Database Group)

Breakout Sessions: Division of Computational Informatics: Computational Media Group

Reviewer: Bruce H. Thomas Room: SB-1111

START	END	SPEAKER	TOPIC
14:00	14:15	Y. Kameda	Introduction
14:15	15:35	Y. Kameda / I. Kitahara	Research Result 1
			Visual Exploratory Activity for Read-The-Game Skill Evaluation of Football Players and for Behavioral Analysis under Microgravity Conditions Image Based Location Estimation for Walking Out of Visual Impaired Person Walkable Area Estimation for Visually Impaired Swimmer Position Estimation by Lane Rectification Others and Future Plan
15:35	15:50		COFFEE BREAK
15:50	17:10	I. Kitahara	Research Result 2
			Multi-Resolution Bullet-Time Effect Smoothly Switching Method of Asynchronous Multi-view Videos Using Frame Interpolation On-site Visual Feedback Method Using Bullet-Time Video MR Visualization of Wheel Trajectories of Driving Vehicle by Seeing-Through Dashboard A Projector Calibration Method Using a Mobile Camera for Projection Mapping System Others and Future Plan
17:10	17:25		COFFEE BREAK
17:25	17:55	H. Shishido	Research Result 3
			Calibration of multiple sparsely distributed cameras using a mobile camera Proactive Preservation Activity of World Heritage by 3D Reconstruction Technology Others and Future Plan
17:55	18:10	Y. Kameda	Fundings and Collaborators
18:10	18:15		SHORT BREAK
18:15	18:30	Y. Kameda	Concluding Remarks

Y. Kameda (Computational Media Group)

21th February (Friday)

<u>Activities of Divisions (cont'd)</u> (**Workshop Room**)

10:00-10:15 Promotion Office for Computational Sciences (D. Takahashi)

10:15-10:30 Liaison Office for Multidisciplinary Computational Sciences (D. Takahashi)

10:30-10:45 The Bureau of Public Relations and Strategy (K. Sekiya)

10:45-11:00 Coffee Break

11:00-11:30 Future Plan of CCS (T. Boku)
11:30-13:00 Internal Lunch Meeting by External Review Committee
13:00-14:00 Open Discussion and Review Summary

14:00 Closing Remarks (W. Gropp)

D. Takahashi

K. Sekiya

L. Hernquist , M. Sato, W. Gropp, J. Zhang

J. Xu Yu, B. H. Thomas, C. Sachrajda,
H. Nakashima, P. Maris

Report of the Review Committee

July 24, 2020

Center for Computational Sciences
University of Tsukuba

Member List of the External Review Committee

William Gropp (Chair)	High Performance Computing Systems	Director National Center for Supercomputing Applications, USA
Masaki Satoh (Vice Chair)	Global Environmental Science	Professor Atmosphere and Ocean Research Institute, The University of Tokyo, Japan
Chris Sachrajda	Particle Physics	Professor Department of Physics and Astronomy, University of Southampton, UK
Lars Hernquist	Astrophysics	Professor Harvard-Smithsonian Center for Astrophysics, Harvard University, USA

Pieter Maris	Nuclear Physics	Professor Depertment of Physics and Astronomy, Iowa State University, USA
Angel Rubio	Quantum Condensed Matter Physics	Director, Max Planck Institute for the Structure and Dynamics of Matter, Germany & Distinguish Research Scientist, Center for Computational Quantum Physics, Flatiron Institute, USA
John Zhang	Life Sciences	Professor, NYU-ECNU Center for Computational Chemistry, New York University Shanghai, China
Shiguang Miao	Global Environmental Science	Director, Institute of Urban Meteorology, China Meteorological Administration, China
Hiroshi Nakashima	High Performance Computing Systems	Professor, Academic Center for Computing and Media Studies, Kyoto University, Japan
Jeffrey Xu Yu	Database	Professor, Department of Systems Engineering and Engineering Management, Chinese University of Hong Kong, Hong Kong
Bruce H. Thomas	Computational Media	Professor, School of Information Technology and Mathematical Sciences, The University of South Australia, Australia

1 Overall Summary 総論

The review of the Center for Computational Sciences at the University of Tsukuba was conducted with on-site presentations and discussions in the period February 19-21, 2020. Shortly after this, the COVID-19 pandemic forced many of the committee members into a lockdown, which impacted the committee's efforts to complete this written report and finish its recommendations. The committee emphasizes that the delay in completing this report was solely due to the challenges created by the pandemic.
We thank the scientists and staff of the CCS for their hospitality and their arrangements for the review which greatly assisted us in our task of assessing the activities and preparing this report. We thank everyone for giving simple and clear answers to the various questions we posed and for explaining their opinions and ideas. We enjoyed the array of new and developing science shared with us through talks, posters and laboratory visits. The organization of our visit was first rate and it was a pleasure to participate in this External Review Board.

筑波大学計算科学研究センターの外部評価は 2020 年 2 月 19 日から 21 日かけて、同センターにおいて行われた。その後、COVID-19 禍による行動制限等に影響されたが、外部評価委員の努力によって本報告書が完成された。委員会としては、この報告書作成の遅延はひとえに COVID-19 感染症拡大によって引き起こされたということを強調しておきたい。

外部評価委員会は、本評価における計算科学研究センター研究者の多大な調整やサポートが、本報告書の完成に大きな助けになったと考えている。我々は、多くの質問に対しシンプルかつ的確な回答を出してもらい、また彼らの意見や考えを丁寧に説明してくれたことに感謝する。彼らとの議論及びポスター展示や研究室見学を通じ、多くの科学的アイデアや研究推進に関する知見を共有できた。我々の訪問に対する対応を非常に高く評価したく、また今回の外部評価委員会に参加できたことは我々として大きな喜びである。

1.1 Summary of Conclusions and Recommendations 結論及び提言のまとめ

1) The Review Committee was impressed overall by the work of the Center for Computational Sciences (CCS), the interdisciplinary culture, leadership, activities since the last review, and vision for the future. The committee believes that the center, with its strong coupling of applications and computer science code development and successful collaborations, has created a unique research environment. The CCS has developed and been a leading proponent of the design of computer system in partnership with applications, an approach now called "co-design". This approach is necessary for advancing computational capabilities, especially after the end of Dennard Scaling. The CCS has a long history of developing, building, and deploying high-performance computing (HPC) systems. The Cygnus computer system is a great example of the innovative work of CCS in exploring new concepts and ideas for addressing the limitations of current computer architecture approaches, which can only be accomplished in a center where applications and computer science work closely together. CCS serves

as an example of interdisciplinary computational science research, and this should continue to both strength current activities and build more collaborations. Since the last review, new areas in life sciences and health research are good examples of the benefits of interdisciplinary collaboration and should be continued. To continue as a world-leading research center, the CCS will need to attract new researchers, addressing needs for both more diversity and, in some areas, early and mid-career researchers. The Review Committee commends the CCS to the University and recommends that the University acknowledge the strategic value of the CCS, support the execution of its mission, and encourages the wide academic community to engage with its activities.

外部評価委員会（以下、「委員会」）は、計算科学研究センター（以下、「CCS」）における前回の外部評価から現在に至るまでの学際計算科学の文化、リーダーシップ、研究活動、今後の発展に対するビジョン等の進歩に感銘を受けた。委員会は、CCS における応用分野と計算機科学分野の強力な協業によるプログラム開発や共同研究関係が、同センターの特徴的な研究体制を形成していると信じる。CCS は、今日 co-designing（協調設計開発）と呼ばれるようになった、アプリケーション側との協業による計算機システム設計の先駆者でありそのリーダーシップを取り続けている。このアプローチは、特にデナードスケーリングの終焉が近い現在、計算性能の向上に必要不可欠である。CCS は高性能計算（HPC: High Performance Computing）システムの設計・開発・実用に関する長い歴史を持つ。Cygnus システムは現在のスーパーコンピュータのアーキテクチャ的限界を打ち破る新しい概念とアイデアを取り込んだ画期的なシステムであり、これは応用科学者と計算機科学者の密接な協業という体制の下でしかなし得ない成果である。CCS は学際計算科学研究の具体例であり、現在の体制の維持とより発展的な共同研究は継続されるべきである。前回の外部評価以降、生命科学や健康科学といった新分野の研究の立ち上げは学際計算科学の成果であり、今後も継続されるべきテーマである。今後、CCS が世界トップレベルの研究を継続するためには、新しい研究者の登用、特に性別や人種にとらわれず、分野によっては若手や中堅の研究者を積極的に採用すべきである。委員会は、筑波大学に対して CCS の活動支援を推奨すると共に、大学が CCS の戦略的価値を評価し、彼らのミッションを支援し、彼らの研究が広い科学分野において発揮されるよう援助することを進言する。

2) The CCS has eight research divisions, each of which has a strong record and good future plans. Applications are the focus of six of these divisions, and cover topics in particle physics, astrophysics, nuclear physics, quantum condensed matter physics, life sciences, and global environmental science. The work of these divisions is in general excellent. A strength of many of these research efforts is the integration with the Computer Science and HPC research efforts.

   CCS は 8 つの研究部門を持ち、それぞれの部門は素晴らしい成果と良好な将来計画を持っている。うち 6 つの部門は、素粒子物理、宇宙物理、原子核物理、量子物性、生命科学、地球環境科学の各応用分野を対象としている。これらの分野における研究は全般的に優れている。これらの研究の多くは計算機科学研究者との共同研究と HPC 研究の努力によって支えられている。

3) The other two divisions are in the areas of computer and computer systems research. These include computational informatics (with two groups, in database and

computational media) and high-performance computing systems. The work of these divisions is in general excellent, and has an effective balance between basic and applied research.

その他の 2 つの研究部門は計算機科学分野に属する。それらは計算情報学（さらにデータ基盤と計算メディア工学の 2 分野に分かれる）と、高性能計算システムに関するものである。これらの部門の研究は全体的に優れており、基礎と応用の両面に渡る良好なバランスを保っている。

4) These divisions demonstrate excellence within their disciplines and their senior members are leaders of successful projects of the CCS.

   これらの研究部門においては、研究者らの努力と、指導的立場にいる研究者のリーダーシップによって、CCS における各種の素晴らしい研究成果が生み出された。

   a) Research in the **Division of Particle Physics** is centered around Lattice Quantum Field Theory in general and in the exploitation of Lattice Quantum Chromodynamics (QCD) in particular. The group is very well known internationally. It continued to execute a wide-ranging and interesting programme of research in Lattice Field Theory in the review period and has an exciting future program in three areas: (i) the exploitation of the PACS10 configurations, (ii) QCD dynamics at finite temperature and density and (iii) in the application of the Tensor Network scheme. The master field simulations on large lattices at the physical point are unique, and we look forward to seeing the scientific return from this very impressive investment, an investment that is particularly appropriate for a division of the CCS, in the near future.

      素粒子物理研究部門における研究は、格子上の量子場の理論を中核としており、特に格子量子色力学(QCD)において先駆的である。筑波大学を中心とした本グループの名声は世界的に広く知れ渡っており、今回の評価期間における格子上の場の理論の研究においても、幅広く且つ興味深い研究プログラムが遂行されている。また、将来的にも(i)PACS10 配位を用いた物理量計算、(ii)有限温度・有限密度下における QCD ダイナミクスの研究、(iii)テンソルネットワークスキームの格子上の場の理論への応用、の 3 つの領域において刺激的な研究プログラムが用意されている。特に、超大体積格子を用いた物理点でのマスターフィールドシミュレーションは独創的な研究であり、この非常に野心的な試みがもたらす科学的成果に期待している。今後の短期的な展望として、本部門がマスターフィールドシミュレーションによる物理研究を遂行していくことはとりわけ時宜を得ている。

   b) The **Division of Astrophysics** has been conducting research and providing world-class leadership in nearly all of the most important topics in the field. This includes the formation of supermassive black holes in galaxies, the growth of large-scale structure in the Universe, galaxy formation, feedback from supermassive black holes and supernovae, accretion onto neutron stars and black holes, and galactic dynamics. The group has also been very active in developing and implementing novel algorithms for performing radiative transfer and solving the equations of magnetohydrodynamics in a general relativistic context. Cross-cutting programs include the codesign of hardware and algorithms, astrobiology, and optical biomedical imaging.

宇宙物理研究部門は、宇宙分野におけるほとんど全ての最重要課題について研究を展開し、世界第一級のリーダーシップを発揮している。その研究テーマは、銀河の超巨大ブラックホール形成、宇宙大規模構造の成長、銀河形成、超巨大ブラックホールおよび超新星からのフィードバック、中性子星やブラックホールへの降着、銀河力学にわたっている。さらに、この部門では、輻射輸送計算や一般相対論的磁気流体力学を解くための新たなアルゴリズムの開発と実装を非常に精力的に行ってきた。そして、異分野連携として、計算機ハードウェアやアルゴリズムのコデザイン、宇宙生命、医用光学イメージングも進めている。

c) The **Division of Nuclear Physics** performs forefront theoretical and computational research for nuclear quantum many-body systems. The Division has a good publication record, is successful in securing grant support, and three of its junior members received young scientist awards. The group uses time-dependent Density Functional Theory to study phenomena such as nuclear fission, reactions, and collective motion in nuclei. Similar methods are also used in condensed matter physics and the CCS allows for fruitful cross-fertilization between these two divisions. The group makes excellent use of the available computational resources and benefits from the HPC expertise within the CCS; this connection could be further enhanced in the future. Other projects include investigations of the role of nuclear structure in double beta decay, and the ImPACT project "Reduction and Resource Recycling of High-level Radioactive Wastes through Nuclear Transmutation". The latter resulted in an open website that is an excellent example of outreach to the general public about nuclear physics.

原子核物理研究部門では、原子核量子多体系に対して最先端の理論計算を用いた研究が行われている。優れた成果出版履歴を有しており、研究遂行に十分な外部資金の獲得にも成功している。また、本部門の研究者に指導を受けた大学院生等 3 名が、若手サイエンティストに対する賞を受賞している。本部門では、時間依存密度汎関数理論を用いて、原子核の核分裂、核反応、および集団運動などの現象を対象にした研究を実施しているが、類似した手法は、凝縮系の物理においても使われており、センター（CCS）は、これら２つの部門間の実りある相互交流の機会を提供している。また、センターにおいて利用可能な計算機資源や、ハイパフォーマンス・コンピューティング（HPC）の専門的経験をうまく利用することで成果をあげている。この連携は将来さらに強力にすることができるであろう。その他のプロジェクトとして、二重ベータ崩壊における核構造効果の研究、ImPACT プロジェクト「核変換による高レベル放射性廃棄物の大幅な低減・資源化」などがあり、特に後者では、ウェブサイトを公開し、原子核物理学を一般大衆向けに解説した素晴らしいアウトリーチの一例となっている。

d) The **Division of Quantum Condensed Matter Physics** has pushed forward in the last five years the promotion of “Multidisciplinary Computational Science,” benefiting from a clear cross fertilization between the specific scientific goals in each division and the development of high performance codes and software that benefits from the new computational infrastructures combining GPU, CPU and FPGAs. The division continues to develop top-level software that is widely used by the whole international scientific community (in particular the SALMON code developed by Yabana's group in close collaboration with Boku's group its having a major impact). This synergetic collaboration led to impressive scientific results on the modelling and simulation of complex dynamic processes away from equilibrium and ultrafast time-resolved spectroscopies steming from the massive improvements made in the performance. The code is really at the forefront of the international research field on the description of ultrafast and non-equilibrium phenomena in atomic, molecular and solid-state physics. Strengthening this division as a prime research unit and fostering synergy with other units is a must and the committtee recommends reinforcing the human resources of the unit (see the section on personel below).

量子物性研究部門ではこの 5 年間、各部門の科学面での目標と、GPU、CPU、FPGA を組み合わせた新しい計算基盤を活用した高性能なコードやソフトウェア開発との明瞭な融合を活用することにより、「学際計算科学」を推進してきた。当部門では、全世界にわたる科学界で広く利用されているトップレベルのソフトウェアの開発を継続している（特に矢花グループと朴グループの緊密な連携により開発した SALMON コードが主たるインパクトを持つ）。このような協働により大幅なパフォーマンスの向上が実現し、平衡から離れた複雑な動的過程や超高速時間分解分光のモデリングやシミュレーションに関する優れた科学的な成果が得られた。このコードは実際、原子・分子・固体物理学における超高速・非平衡現象の記述に関し、国際的に最先端のものとなっている。本部門を中核的な研究ユニットとして強化し、他のユニットとの相乗効果を高めることが必要であり、委員会は本部門の人材強化を推奨する（後述の人材に関する節を参照）。

e) The **Division of Life Sciences** is prominent, visible and highly productive in computational bimolecular science, eukaryotic phylogeny and evolution. The division's research spans a wide range topics including QM/MM studies of enzymatic reactions, developing enhanced sampling methods for molecular dynamics, development of GPU-accelerated software, Global eukaryotic phylogeny and Evolution of mitochondria, etc. The groups have made significant advances in their research areas and are recognized by their peers. Their research involves a combination of theoretical and computational approaches across the field of physics, chemistry, biology, material, bioinformatics and high-performance computing. They have established extensive intra- and inter-institute as well as international collaborations. The Division has published many high-quality research articles and is very successful in securing research grants. The Division is super active and research productive.

生命科学研究部門は、計算生体分子科学、真核生物の系統形成と進化の分野で顕著、かつ目に見える形で非常に生産性の高い研究を行っている。特に酵素反応の QM/MM 研究、分子動力学のための高度なサンプリング法の開発、GPU ソフトウェアの開発、真核生物の系統解析とミトコンドリアの進化など、幅広いテーマで研究を行っている。２つの研究グループは、それぞれの

研究分野で大きな成果を上げており、世界中の研究者からも認められている。しかも物理学、化学、生物学、材料学、バイオインフォマティクス、高性能計算の融合分野において、理論的アプローチと計算機的アプローチを組み合わせた学際的研究を行っている。また、研究所内、研究所間、国際的な共同研究を幅広く展開している。当部門は、多くの質の高い研究論文を発表しており、また研究助成金の獲得にも成功している。以上のように、この部門は極めて活発で、さらに研究生産性が高いと結論づけられる。

a) The **Divsion of Global Environmental Science** is making very strong contributions to the CCS, working on relevant topics (including computationally intensive science), collaborating with relevant groups (including the CCS Division of Computational Informatics and the Division of High-Performance Computing Systems), performing fore-front work within their area of expertise, and educating impressive numbers of students. The division's intensive research fields are urban climatology, mountain meteorology, atmospheric general circulation, and predictability with using computationally intensive high-resolution global and regional models, together with the large eddy simulation (LES) model. The archive of the unique meteorological datasets is well received by the research community. Thanks also to international collaborations and domestic research networks, by any measure, they are doing an excellent job.

地球環境研究部門は、関連するトピック（計算科学）に取り組み、関連するグループ（計算情報学部門および高性能計算システムの部門）と協力して、CCS に非常に大きな貢献をしている。彼らの専門分野における最前線の研究と非常に多数の学生の教育を行っている。この部門の主な研究分野は、高解像度グローバルモデル、地域モデル、ラージエディシミュレーション（LES）モデルを用いた都市気候学、山岳気象学、大気大循環、および、予測可能性の研究である。独自の気象データセットのアーカイブは、研究コミュニティから好評を得ている。また、国際的な協力と国内の研究ネットワークにより、彼らは素晴らしい仕事をしている。

b) The **Division of High Performance Computing Systems** has excellence not only in their research work but also in the deployment and operation of CCS's HPC systems, HA-PACS, COMA, Oakforest-PACS and Cygnus, which have acted as the main computational facility of CCS and is a key component of Japan's HPCI. As for their architectural research, recent accomplishments in FPGA/GPU-hybrid architecture, which is realized in Cygnus, shows us its high potential, especially in low-latency and high-bandwidth communication. Their software work is highly appreciated not only for the many excellent publications but also the fact that the research is based on their own software products, Gfarm files system, Pwrake workflow system and FFTE library.

高性能計算システム研究部門は彼らの研究分野における成果だけでなく、CCS における HA-PACS, COMA, Oakforest-PACS, Cygnus といった歴代のスーパーコンピュータの導入と運用にも貢献しており、これらのシステムは日本における HPCI（High Performance Computing Infrastscutre：革新的ハイパフォーマンス・コンピューティング・インフラ）における重要な資源となって

いる。彼らの計算機アーキテクチャに関する研究は、最新の FPGA と GPU をハイブリッドに組み合わせたシステムとして Cygnus を生み出し、その潜在的性能に加え、低いレイテンシと高いバンド幅を持つ通信ネットワークを実現した。彼らのソフトウェア開発力は称賛すべきであり、多くの優秀な論文の発表につながっただけでなく、Gfarm ファイルシステム、Pwrake ワークフローシステムや FFTE ライブラリ等の実用的システムを生み出している。

c) The **Division of Computational Informatics** is one of strongest teams on database research in Japan, nation-wide. This Division serves an important role in the center under the mission of "multidisciplinary computational science" with a focus on big data analytics and AI to support large applications that need highly efficient data processing techniques. On the one hand, the Division has focused on information integration framework, data mining and knowledge discovery, and provided new techniques to address real issues via collaboration with specialists in different application domains. On the other hand, the Division has explored new techniques using advanced hardware such as GPU and FPGA. The Division has many papers published in major international conferences and renowned journals, and received 14 awards including 8 best paper awards in the past 6 years.

計算情報学研究部門は、データベース研究において日本国内で最も強力なチームの一つである。同部門はセンターがミッションとする学際計算科学のもと、ビッグデータやAIにフォーカスし、高度に効率化されたデータ処理技術を必要とする大規模アプリケーションをサポートする上で重要な役割を果たしている。同部門は、情報統合フレームワーク、データマイニング、知識発見に焦点を当て、様々なアプリケーション分野の専門家とも協力しながら、実問題の解決を目指した新たな技術を提供している。一方、同部門は、GPUやFPGAといった新たな先進的ハードウェアを用いた新たな技術も開拓している。同部門は主要な国際会議や著名なジャーナルに数多くの論文を発表しており、過去6年間に8件のベストペーパー賞を含む14件の賞を授与されている。

The **Computational Media Group** is well known for their research in Augmented and Virtual Reality. The areas of research span computer vision, projector-base system, and user interaction. A strength of the group is its strong connections to different parts of the University. The Computational Media Group performs strategic research with real-world impact as a major goal. To perform this form of research, they work closely with scientists in CCS Tsukuba.

計算メディアグループは、拡張現実とバーチャルリアリティの研究でよく知られている。研究分野は、コンピュータビジョン、プロジェクターベースシステム、およびユーザーインタラクションに及ぶ。本グループの強みは、大学の異なる分野との強い連携である。計算メディアグループは、現実世界へインパクトを与えられる戦略的研究を、主目標としている。こうした研究を行うために、CCS 内の研究者と密接に協力して研究を進めている。

2) The CCS has a long history using information about the computational needs of applications in designing and configuring high performance computing systems. This approach is now called "co-design," and is widely used to address the increasing

challenges in increasing computational power with the end of Dennard (frequency) scaling of processors. The committee finds the current work of the CCS in co-design, especially the combination of FPGAs and GPUs, to be innovative and responsive to the needs of applications. The committee also notes that FPGA technology, while promising, is challenging to use effectively. The Cygnus system provides a valuable and important testbed in which to explore the potential of this approach.

CCS ではこれまでの活動において、応用側研究者の様々なニーズに基づき、高性能計算システムの構築を行ってきた。このアプローチは現在は co-designig と呼ばれており、デナード則（周波数）によるプロセッサの性能限界が見えている中で、さらなる高性能化を目指す上で必要とされている概念である。委員会は、現在の CCS における co-designing について、特に FPGA と GPU の併用はアプリケーションの性能要求に対する革新的な対応として評価する。さらに委員会は、FPGA は有望な技術であるが、これを実際に応用に適用することは必ずしも容易ではなく、それ自体は大きなチャレンジであると考える。Cygnus システムは、このアプローチにおける潜在的な可能性・有望性を含んでおり、そのための重要な環境を提供している。

3) The committee is impressed with the supercomputer facilities and their usage and support for the research community in Japan. The committee supports the plans for PACS-XI and the Post-OFP with the University of Tokyo.

   委員会は、スーパーコンピュータの提供とその運用が日本における研究コミュニティを強力に支援していることに感銘した。委員会は、筑波大における PACS-XI プロジェクトと、東京大学との共同研究による Post-OFP（Oakforest-PACS 後継システム）の計画を支持する。

4) In the 2014 review, the panel recommended the CCS to strengthen and expand their international exchange program for scientists, as well as establishing an exchange program for students. In response to these recommendations, the CCS expanded their support for international meetings and schools, long-term visitors, as well as monthly sabbatical leaves. Since 2014, there have been joint annual workshops with the Edinburgh Parallel Computing Centre (EPCC) and with the Lawrence Berkeley National Laboratory (LBNL). In addition, also since 2014, there have been joint Japan-Korea HPC winterschools. This is an excellent way to build collaborations between the CCS and other world-leading research groups, and the committee recommends continuing these activities and expanding them if possible. The committee also supports creating additional opportunities for international students to intern at the CCS.

   2014 年における外部評価では、CCS が研究者及び学生の国際的交流を推し進めるよう提言した。これらの提言に基づき、CCS は各種国際的なワークショップ、スクール、長期招聘、マンスリーサバティカル等の国際交流活動を展開している。2014 年以降、彼らは英国エディンバラ大学並列計算センター（EPCC: Edinburgh Parallel Computing Center）、米国ローレンスバークレー国立研究所（LBNL: Lawrence Berkeley National Laboratory）のそれぞれとの定例共同ワークショップを毎年開催している。さらに 2014 年以降、韓国と共同で日韓 HPC ウィンタースクールを毎年開催している。CCS が世界中のトップクラス研究所と交流しているこれらの活動について、委員会はこれを継続し、さらに発展させることを提言する。また委員会は、CCS が国際的インターンシップ学生を積極的

に受け入れるよう勧める。

5) The committee finds that the CCS has made substantial contributions to the research community. These include numerous publications, many in leading journals, as well as software and some datasets. The contributions of the HPC systems, both the "production" system Oakforest-PACS, and the experimental system Cygnus, are also significant.

   委員会は、CCS が研究コミュニティにおいて大きな貢献をしていることを認識した。多数の学会発表と雑誌論文発表に加え、様々なソフトウェア開発やデータベースの提供による貢献が大きい。主力計算資源として貢献する Oakforest-PACS と、先進的実験システムとしての Cygnus という 2 つのスーパーコンピュータの提供は重要な貢献である。

6) The committee commends the CCS on its publicity and public outreach activities. These are of high quality. The CCS should look at growing the breadth of impact of their publicity and outreach activities.

   委員会は CCS の質の高い論文出版とアウトリーチ活動を称賛する。CCS はこれらの活動を一層強力に進めるべきである。

7) The committee makes the following observations and recommendations, which apply to more than one division. Other recommendations for the individual divisions are included in the in-depth commentary on each division.

   委員会は以下に述べる観察と提言を、複数の研究部門に跨る活動に対して行った。各研究部門に対する個別の提言は、それぞれの詳細報告の中に記述する。

   a) A strength of the CCS is the close interaction and collaboration between the application groups and the computer science experts. However, some divisions could work more closely with those groups in the CCS. The committee recognizes that the computer science expertise is a limited resource – there aren't enough HPC researchers to continuously work closely with all six application divisions. The committee recommends ensuring that all six application divisions have an opportunity to collaborate closely with the HPC researchers.

      CCS の研究力の強みは、応用科学分野と計算機科学分野の強い共同研究によって提供されている。しかし、いくつかの研究部門は今以上に強く、計算機科学研究グループと協業できるはずである。委員会は、計算機科学側の人的資源は限られており、それらの研究者が応用側の 6 つの研究部門と共同研究を行うには十分でないと考える。委員会は、これらの応用側研究部門がより一層強く、HPC 側の研究者と協調することを推奨する。

   b) While the scientific work is of very high quality and much of it has had great impact in the respective fields, the scientific impact of some groups has been uneven. The committee recommends that the CCS leadership review the research directions and both the expected and achieved impact of research projects to ensure that these efforts are providing the maximum impact for the effort invested. In some cases, this may require better aligning projects to their unique strengths.

      非常に質が高く、影響力の大きい科学的研究成果が複数の分野でなされてい

る一方、いくつかのグループのそれは不十分である。委員会は、CCS が各研究の方向性について、各プロジェクトに期待される成果と影響力について、それらの努力の注力に値する最大の成果が得られるように、CCS の執行部が努力することが必要であると考える。いくつかの分野では、研究者の特徴的な研究対象に沿ったプロジェクトの遂行が必要である。

c) The committee recommends that efforts be made to improve gender diversity and to address age-imbalance among the researchers in several of the groups.

委員会は、いくつかの研究グループにおいて、研究者の性別及び年齢分布のバランスが不十分であり、一層の改善が必要であると考える。

1.2 Major projects and programs

主要プロジェクトとプログラム

Oakforest-PACS and JCAHPC
The committee recognizes Oakforest-PACS as CCS's biggest contribution in its mission of deployment and operation of its own supercomputer systems. It is specially remarked that Oakforest-PACS was ranked Japan's #1 in the Top500 list of November 2016 with HPL performance of 13.6 PFlops, and had kept that position in two successive list publications. In addition, a significantly large portion of its computing capacity has been provided to Japan's HPCI project to make it the largest resource provider in the project after the retirement of K-computer. These accomplishments are considered as the proof of successful collaboration with The University of Tokyo, with which JCAHPC was established as Japan's first and only HPC organization operated by multiple universities. The committee expects that JCAHPC will continue its work for the successor of Oakforest-PACS.

Oakforest-PACS と JCAHPC
委員会は、独自のスーパーコンピュータ資源である Oakforest-PACS の導入と運用において、CCS の貢献が非常に大きいと評価する。Oakforest-PACS が 2016 年 11 月版の TOP500 リストにおいて、HPL ベンチマーク性能 13.6PFlops をもって国内最高性能システムとランクされ、その後 2 回の同リストにおいてその位置を保っていることは特筆に値する。さらに、この巨大なシステムの大きな資源量が、京コンピュータの運用停止後、日本の HPCI プログラムにおいて最大の資源提供元となっていることも特筆すべきである。この事実は、東京大学と共同運営される JCAHPC（Joing Center for Advanced HPC：最先端共同 HPC 基盤施設）での共同活動が、非常に重要なものであることも示している。これは日本における初めての 2 大学によるスーパーコンピュータの共同設置・運用事例である。委員会は、JCAHPC が継続され、Oakforest-PACS の後継システムが実現することを期待する。

Cygnus

The committee respects the uniqueness of Cygnus whose 32 out of 80 GPU-rich nodes, named Albireo nodes, are enhanced by adding two FPGAs to each node and connecting them to form a 2-dimensional torus interconnect. The committee understands that one-year research experiments with Albireo nodes are mostly pursued in computer science side focusing on fundamental FPGA-GPU and FPGA-FPGA communications, but hopes various applications of CCS's own research will find efficient implementations to exploit the high potential of FPGA as the preliminary study with ARGOT showed its effectiveness in small-size problems.

Cygnus
委員会は、Cygnus システムが、GPU を多数搭載した 80 ノードのうち 32 ノード（Albireo と名付けられている）に各 2 基の FPGA を搭載し、それらを 2 次元トーラス結合しているユニークなシステムである点を評価している。委員会は、主として計算機科学研究者グループがこの 1 年間で FPGA-GPU 通信システムと FPGA-FPGA 通信システムの基本部分を開発したことを承知しているが、先進的研究である ARGOT コードの FPGA 対応が小規模問題に有効であることが示されたことをきっかけに、多くの独自開発プログラムでその性能が発揮されることを期待する。

Department of Computational Medical Science
The Department of Computational Medical Science described four projects that it is conducting. Each of these projects involves one (or more) CCS researchers: computational drug discovery, by the Division of Life Sciences, sleep big data analysis by the database group of Computational Informatics, 3D surgical navigation system by the Computational Media group of Computational Informatics, and computational optical bio-imaging by the Division of Astrophysics. Each of the projects is done in collaboration with outside academic, medical, and/or industry collaborators. They are all good examples of interdisciplinary research projects, involving both domain scientists (sometimes from more than one domain) as well as computational scientists. They all address real-life medical science issues, such as enhancing diagnostic tools or development and improvements of medical treatments. The committee strongly encourages such collaborations, and an interdisciplinary research center such as the CCS should be an ideal environment to foster such collaborations.

計算メディカルサイエンス事業部
計算メディカルサイエンス事業部では、4 つのプロジェクトを推進している。各プロジェクトには、一人（ないし数人）の CCS の研究者が入っている。計算創薬は生命科学研究部門、睡眠ビッグデータ解析は計算情報学研究部門データ基盤分野、3DCG バーチャル手術は計算情報学研究部門計算メディア分野、計算光バイオイメージングは宇宙物理研究部門で推進されている。各プロジェクトは、学外の学術機関、医学分野、ないし産業界の研究者との協働で進められている。これらのプロジェクトは全て、ある領域の研究者（場合によっては複数領域の研究者）と計算科学者を含み、学際的な研究プロジェクトの好例となっている。プロジェクトは全て、診断機器の改良や医療の発展・改善など、現実的な医学の問題に取り組んでいる。評価委員会は、このような協働を強く支持する。そして、CCS のような学際的な研究センターは、このような協働を育むのに理想的な環境といえる。

However, it is unclear what the status of this 'Department' is within the CCS. It is not a Research Project, nor a Research Division, nor a support office. In the written documentation it is listed under the ‘Research Project Offices,’ yet in the chart used in the presentations (e.g., slide 5 of the presentation on Activities and Results 2014-2019) it is listed as its own entity, with its own color. The committee strongly recommends continuing these types of interdisciplinary research projects, involving CCS scientists and scientists from other departments and/or other universities, as well as industry partners for actual applications, and the committee recommends that the CCS continue to foster an enviroment in which such collaborations are not only possible, but are actively encouraged.

しかし一方で、CCS の中で“事業部”の位置づけは明確ではない。これは、研究プロジェクトでもなく、研究部門でもなく、推進室でもない。文書の中では、研究開発推進室の一つとしてリストされているが、プレゼンファイルの組織図（例えば、プレゼンファイル Activities and Results 2014-2019 の 5 ページ目）では、独自の位置づけと色付けになっている。評価委員会は、CCS の研究者と他学部や他大学の研究者、さらには実応用の産業界の協力者からなる、このようなタイプの学際的研究プロジェクトの継続を強く奨励するものであり、CCS には、このような共同研究を単なる一つの可能性という以上に、強く支援する環境を継続していただきたいと考える。

ILDG/JLDG project

The nature of Lattice QCD computations is such that some of the computationally intensive elements, in particular the gauge field configurations can be saved and reused for a wide variety of projects in particle physics. The International Lattice Data Grid (ILDG) and Japanese Lattice Data Grid (JLDG) are facilities which successfully enable researchers to access existing stored configurations and hence to maximise the scientific return on the computational investment. The CCS, through it expertise in the Divisions of High Performance Computer Systems, Computational Informatics and Particle Physics, is playing the leading role in JLDG and acts as a representative of the Japanese grid on ILDG. The External Review Committee strongly endorses this activity.

ILDG/JLDG プロジェクト

格子 QCD 計算の特徴として、ゲージ場の配位(訳注：モンテカルロサンプル)の生成にはとりわけ大きな計算コストが必要となるため、配位そのものを保存・共有し、素粒子物理研究の幅広いプロジェクトにおいて再利用するというシステムが構築されている。国際格子データグリッド(ILDG)と日本格子データグリッド(JLDG)は、このシステムを運用・管理している国際的または国内の組織であり、研究者が保存されている配位にアクセスし、それを用いた計算を行うことによってなるべく少ない計算量で最大限の科学的成果を引き出すことを目的としている。CCS は、高性能計算システム研究部門、計算情報学研究部門、素粒子物理研究部門の異分野間連携のもと、JLDG において主導的役割を果たし、ILDG における日本グリッドの代表を務めている。外部評価委員会は本活動を強く支持する。

The committee notes the successful activities to upgrade and maintain the JLQCD system hardware and software since 2014, including improvements in the reduction of the corruption of data in storage and transmission (md5sum checksum), the improved control achieved through the updates of supporting servers and network and the increase in disk space from 2.4PB in 2014 to 13.0 PB in 2020. We recognise the issues highlighted in the report which will need to be tackled in the near future and trust that the necessary budgets and staff will be secured to maintain the operations and to replace some of the basic software which is becoming obsolete. The CCS is very well placed to play a leading role in the reconsideration of the optimal way to share QCD data internationally, particularly as the ILDG activity has been decreasing in the last few years.

本評価委員会は、2014 年以降の JLDG システムのハードウェア・ソフトウェア両面における性能改善・維持管理が首尾良く行われていると考える。例えば、保管や転送におけるデータ破壊の機会の更なる削減(md5sum checksum)、サーバやネットワークに対するサポートの改善によるシステム管理の向上、2014 年〜2020 年における 2.4PB から 13.0PB へのディスク容量の拡張、などが挙げられる。本評価委員会は、重要な短期的検討課題として、システムの安定的な維持・運用および時代遅れとなりつつある幾つかの基本ソフトウェアの更新のために予算と人員の確保が必要だと考える。近年 ILDG の活動は低下傾向にあるが、CCS が QCD 配位の国際的な共有に対する最良の方法を再検討する主導的役割を果たすことが期待される。

In the 2014 review, the committee strongly endorsed the plan to provide the configurations with a DOI number to better trace the usage of configurations and record publications where these configurations were used. We note that in January 2020, the DOI working group of the JLDG team finalised the “terms and agreements” and “procedures” for DOI assignments and that the first assignment of DOI to a JLDG public QCD ensemble will be performed soon.

2014 年に行われた外部評価では、配位の利用履歴の追跡や研究成果の出版実績の取り纏めが容易になることから、配位に対して DOI を付与する計画が当時の評価委員会によって強く支持されている。本評価委員会は、2020 年 1 月時点において JLDG チーム内の DOI 作業部会が配位の DOI 登録に関する合意事項および手続きに関する規約を完成させ、近々JLDG における公開済み QCD 配位に対する最初の DOI 登録が実施される予定であることを確認した。

Multidisciplinary Cooperative Research Program (MCRP)

The Multidisciplinary Cooperative Research Program (MCRP) allocates 50% of the computational resources on the CCS systems. Proposals are reviewed by the Cooperative Research Committee, which consists of 24 members (1/3 from CCS, and 2/3 external members) divided over eight domains. Since 2018, the application is online, and since 2019 open for foreign researchers. Over the past 6 years, the number of proposals has more than doubled from 41 in 2014 to 84 in 2020, spread over the different fields. Data and statistics on effective usage was not available, but the CCS plans to improve on this — we recommend giving this high priority. The MCRP will also play a role in the allocation process for the next Japanese supercomputer, Fugaku.

学際共同利用プログラム（MCRP）

学際共同利用プログラム（MCRP）は、センターが保有する計算資源の 50%を様々なプロジェクトに配分している。プロジェクト申請書は共同研究委員会で審査され、委員会は 24 名のメンバー（センター内 1/3、センター外 2/3）で構成され、8 つの領域に分かれている。2018 年以降、プロジェクト申請はオンライン化され、2019 年度からは海外研究者にも開かれたものとなっている。過去 6 年間に、申請数は、2014 年の 41 から 2020 年の 84 へと 2 倍以上に増加し、その分野も多岐にわたっている。有効利用に関するデータと統計が十分ではなかったが、センターはこの点を改善する計画であり、我々もこの優先的な実行を推奨する。MCRP はまた、日本の次世代スーパーコンピュータ富岳の資源配分においても一役を担うであろう。

The MCRP also organizes annual multidisciplinary symposia to report on the research performed on the computational resources it provided. Since 2018, these symposia are in English – a development the committee strongly commends. In addition to the allocation of computer resources, the MCRP supports development of new applications for different scientific communities, as well as performance optimization for new architectures. These activities are essential for efficient use of the available computational resources and for the exchange of ideas and experiences with the different HPC platforms.

MCRP では、毎年、学際的シンポジウムを主催し、センターが提供した計算資源によって実施された研究に関する成果報告を行なっている。2018 年以降、これらのシンポジウムは英語で行われているが、この進展を委員会は高く評価する。計算資源の配分以外にも、MCRP は様々な科学的コミュニティにおける新たなアプリの開発支援、および、新しいアーキテクチャーに対するパフォーマンス最適化などを支援している。これらの活動は、利用可能な計算資源の有効利用や、異なる HPC プラットフォームにおける経験とアイデアを交換する上で、非常に重要である。

Exascale Computing System Development Project
Exascale computing (and beyond) will rely on innovations in computer architecture to achieve performance and to address costs, such as electric power. This project office in the CCS continues the approach of co-design with the applications. The focus is on exploiting accelerators such as GPUs and in particular, understanding their limitations and devising innovative ways to address those limitations. The committee commends the CCS for continue to be a leading center for co-design and for the emphasis on extreme scale computing and on developing approaches that may provide HPC systems with better “strong scaling” performance.

次世代計算システム開発室
エクサスケール（またさらにその先）の計算技術は、性能とコストや消費電力を総合的に睨んだ計算機アーキテクチャの革新に大きく依存している。CCS におけるこの研究プロジェクトは、アプリケーションとシステムのコデザインを継続している。特に、GPU のようなアクセラレータをどのように活用するかに着目しており、その技術的限界をどのように超えられるかを模索している。外部評価委員会は、CCS がこのようなコデザインにおける先導的センターとして継続することを望んでおり、より高度な Strong Scaling（一定問題規模における性能拡張）を提供するような超大規模 HPC システム開発を目指してほしい。

Joint Institute for Computational Fundamental Science (JICFuS)
CCS is one of the three founding institutions of the Joint Institute for Computational Fundamental Science (JICFuS); since 2014, JICFuS has eight member institutions. Through JICFuS, CCS plays an active role in providing nation-wide support for computational research, establishing priority computational science projects, and managing allocations for the K supercomputer (retired in Aug. 2019) and for the recently deployed Fugaku supercomputer (world's fastest computer as of June 2020). With its combination of HPC expertise and application science divisions, the CCS is uniquely positioned to support the activities of JICFuS, and to continue playing a leading role in this important national organization.

計算基礎科学連携拠点**(JICFuS)**

CCS は計算基礎科学連携拠点(JICFuS)創設時の 3 機関のうちの一つである。2014 年に JICFuS は 8 機関に拡張された。JCFuS での活動を通して、CCS は国内の計算基礎科学研究に対する支援や、スーパーコンピュータ「京」 (2019 年 8 月運用停止)や最近稼働を開始したスーパーコンピュータ「富岳」(2020 年 6 月時点で世界最速)を用いた重点的計算科学プロジェクトを推進してきた。CCS は、HPC を専門とする計算機科学と計算科学の各部門が協力することによって、JICFuS の活動に対して独自の支援を行うとともに、今後も主導的な役割を果たしていくことが期待される。

2 Research Activities 研究活動

2.1 Division of Particle Physics 素粒子物理研究部門

The research area of the Division of Particle Physics is in Lattice Field Theory in general and Lattice Quantum Chromodynamics (QCD) in particular. In Lattice Field Theory, space and time are approximated by a discrete lattice of points and physical quantities are obtained by numerical simulations. The Division is an internationally recognised group in Lattice Field Theory with a wide-ranging programme of research and many collaborators both within Japan and abroad. It continues to have access to excellent computing resources allowing it to perform extremely CPU-intensive QCD simulations. It is well integrated within the CCS, e.g., it has worked with the HPCS Division on the development of a mixed-precision quark solver for a large Intel Xeon Phi (KNL) system named “Oakforest-PACS” and in developing parallel programs for the Tensor Renormalization Group Methods. The panel has also been impressed with the leading role that the CCS has been playing in maintaining, developing and upgrading the Japan Lattice Data Grid (JLDG), a significant resource for the Japanese lattice researchers, allowing them to access 59 ensembles, generated on a variety of supercomputers, for scientific measurements. The CCS also represents JLDG in the International Lattice Data Grid. We also note the opportunities that will be opened up for further interactions between the physicists in the Division and computer scientists at the Joint Institute for Computational Fundamental Science (JICFuS) of which the CCS is a member. Professor Kuramashi was the Chair of the Local Organising Committee of the 2015 International Symposium on Lattice Field Theory held in Kobe.

素粒子物理研究部門の研究分野は、格子上の場の理論であり、特に格子上の量子色力学(QCD)に重点が置かれている。格子上の場の理論では、空間と時間が離散化された格子点で近似され、数値シミュレーションによって物理量を計算する。本部門は格子上の場の理論の分野において国際的な名声を得ているグループであり、幅広い研究プログラムと多くの国内外の共同研究者を有している。本グループは、優れた計算機資源を用いて多大な CPU コストを必要とする QCD シミュレーションを行っている。高性能計算システム研究部門との共同研究により、“Oakforest-PACS”と名付けられた大規模インテル Xeon Phi(KNL)システム向け精度混合型クォークソルバーを開発し、またテンソル繰り込み群法に対する並列計算コードを開発するなど、CCS 内連携も効果的に行われている。また、本評価委員会は、これまで CCS が日本格子データグリッド(JLDG)の開発・

運用・性能改善において主導的な役割を果たしてきたことに強く印象づけられた。JLDG は日本の格子 QCD 研究者にとって重要な大規模データ資源であり、様々なスーパーコンピュータによって生成された 59 セットものゲージ場配位を提供し、それを用いた科学的計算に貢献してきた。CCS は国際格子データグリッド(ILDG)における日本拠点の代表も務めている。本評価委員会は、CCS が参画している計算基礎科学連携拠点(JICFuS)における活動を通じて、本部門のメンバーと計算機科学者との更なる連携関係の構築に期待している。藏増教授は、2015 年に神戸で開催された格子上の場の理論国際会議の組織委員会委員長を務めた。

The research activities of the Division were presented under 5 headings and we briefly comment on each of these:

本部門の研究活動は 5 つのテーマに大別され、その各々に対するコメントを以下に簡潔に記す。

i) Master field simulation at the physical point in 2+1 flavour QCD: A major focus of the group is the generation of gauge field configurations with the O(a)-improved Wilson quark action and the Iwasaki gluon action with physical light-quark masses on lattices with extent of more than 10fm in each dimensions (the PACS10 gauge configurations). At the time of the review the group had generated such ensembles with lattice spacing a = 0.085 fm and a = 0.065 fm and are currently generating a very fine ensemble with a = 0.041fm. This is a very major undertaking and provides an exceptional opportunity for a major programme of physics exploitation, both in the interesting applications mentioned explicitly in the group's "Future Plans" and hopefully beyond.

i)２＋１フレーバーQCD における物理点でのマスターフィールドシミュレーション: 本研究グループが注力する計算の一つが、O(a)改良された Wilson クオーク作用と岩崎グルーオン作用を用いた物理点における$(10\mathrm{fm})^4$ を超える時空間体積を持つゲージ場配位(PACS10 ゲージ場配位と呼ばれる)の生成である。本外部評価が行われた時点では、格子間隔 a=0.085fm と a=0.065fm のゲージ場配位の生成が終了しており、a=0.041fm の配位は生成途中という段階であった。本計算は非常に重要なプロジェクトであり、生成されたゲージ場配位を用いた物理研究は、従来の計算では得ることが出来なかった卓越した成果をもたらすだろう。既に本グループの将来計画において興味深い物理量計算について記されているが、それを超える成果も期待される。

The early measurements being performed on the PACS10 configurations are all in central areas of research in particle physics. These include: i) the determination of the V_{us} element of the Cabibbo-Kobayashi-Maskawa (CKM) matrix, (needed to test the unitarity of the first row of the CKM matrix); ii) the contribution of the Hadronic Vacuum Polarisation (HVP) to the anomalous magnetic moment of the muon (a quantitative understanding of which is required to compare with the experimental measurement, soon to be updated at FermiLab) and iii) computations of the nucleon's electromagnetic form factor and the determination of the isovector charge radius (which given the proton size puzzle remains important.

素粒子物理学の中心的な研究課題について、既に PACS10 配位を用いた早期の物理量計算が遂行されている。これらの中には、i)Cabibbo-小林-益川(CKM)行列の V_{us} 行列要素(CKM 行列の第 1 行のユニタリティーテストのために必要)、ii)μ 粒子の異常磁気能率に対するハドロン真空偏極(HVP)効果の寄与(米国 Fermi 研究所で近々実験結果の更新が

予定されており、それとの定量的比較のために必要)、iii)核子電磁形状因子の計算とアイソベクトル成分の電荷半径の決定(陽子サイズ問題にとって重要)、などが含まれる。

ii) Hadron-hadron interactions: We are still at the very-very early stages of attempts to perform ab initio QCD computations in nuclear physics (Prof. S. Aoki is a world pioneer in this endeavour). The group has been studying light nuclei since 2010, albeit with very heavy light-quark masses. An interesting study was that of the binding energy deuterium at almost physical quark masses; this is a difficult calculation and, in spite of 10^5 measurements, the noise becomes too large to obtain a result and the group plans to develop new techniques to reduce the statistical error significantly at the physical point.

ii)ハドロン-ハドロン相互作用: 原子核物理における QCD を用いた第一原理計算の試みは、未だ初期とも呼べないほどの未熟な段階である(青木教授は世界におけるその草分けの 1 人である)。本グループは、2010 年から非常に重いクォークを用いて質量数の少ない原子核の直接構成を試みている。物理点近傍での重水素原子核の束縛エネルギーの計算は興味深いが、これは難しい計算であり、10^5 回の物理量計算を実行してもノイズが大きく、統計的に有意な結果が得られていない。今後、物理点において統計誤差を劇的に削減する新たな計算方法の開発が予定されている。

We note that the topics discussed in this subsection are not mentioned in the Division's future plans. This is a little surprising given some of the interesting, but inconclusive, results mentioned in the report, e.g., the group's tantalising results for the $K \to \pi\pi$ decay amplitudes obtained with Wilson fermions and periodic boundary conditions. These are very important processes, but difficult to compute, and it would be very interesting to see whether this project, with a moving kaon can be developed further.

評価用レポートに記載された本部門の将来計画の中に、ハドロン-ハドロン相互作用に関する記述が見当たらないが、この点に関しては少々驚いている。というのも、評価用レポートでは、進行中の段階ではあるが、興味深い計算の途中結果が報告されているからである。例えば、周期的境界条件の下で Wilson フェルミオンを用いて計算された $K \to \pi\pi$ 崩壊振幅では、大変興味をそそられる結果が得られている。これらは難しい計算ではあるが、非常に重要な物理プロセスであり、K 中間子が動いている座標系を用いた計算の更なる展開の可能性は大変興味深い。

iii) Lattice QCD at finite temperature and density: The study of QCD at finite temperature and density is a major global research activity with important applications to astrophysics and cosmology. The HotQCD collaboration, with members from the CCS, is one of the leading contributors to the field and the CCS group itself is making interesting contributions. Among the studies during the review period which have made a particularly strong impact have been the determination of the QCD Equation of State to sixth order in the chemical potentials and the study of the freeze-out pattern and temperature of strange baryons. The successful collaboration within HotQCD is planned to continue with further studies of QCD thermodynamics using the Highly Improved Staggered Quark Action with 2+1 quark flavors with physical masses. An indication of Prof H. Ohno's standing in the community has been the invited plenary talk he gave entitled "Recent progress on in-medium heavy flavor physics from lattice QCD," at the 2019 International Symposium on Lattice Field Theory (Lattice 2019) in Wuhan China.

iii)有限温度・有限密度における格子 QCD: 有限温度・有限密度 QCD の研究は、天体物理学や宇宙論への応用を伴う重要な研究であり、世界各国で行われている。HotQCD collaboration は、CCS からの参加者も含まれており、この分野において主要な貢献を果たしている研究グループの一つである。また、CCS 内の研究グループも独自に興味深い研究成果を出している。今回の評価期間において特に強いインパクトを持つ研究成果は、化学ポテンシャルの 6 次の項まで取り入れた QCD の状態方程式の決定とストレンジバリオンがフリーズアウトするパターンや温度の調査である。これらの成功により、HotQCD collaboration は、今後も高度に改良されたスタッガードクォーク作用を用いて物理点における 2+1 フレーバーQCD のダイナミクスの研究を継続する計画である。大野助教は、2019 年に中国の武漢で開催された格子上の場の理論国際会議において、"Recent progress on in-medium heavy flavor physics from lattice QCD"という題目でプレナリ招待講演を行っており、研究分野のコミュニティから高く評価されていることがわかる。

CCS members, together with colleagues from other institutions in Japan, will also continue their studies of QCD thermodynamics using the gradient flow, building on their successful studies of the Equation of State with unphysically heavy quarks. The next stage will be to extend the study to 2+1 flavors with physical quark masses. They will also continue their investigations into a major challenge for the Lattice QCD community, establishing the phase diagram of QCD in the temperature-chemical potential plane, extending their Wilson fermion studies from 3-degenerate quarks to 2+1 and 4 flavors (and studying the universality by comparison with results from staggered quarks). In the three flavor study they were able to obtain the temperature at the critical end-point, T_E = 134(3) MeV.

CCS の研究者は、国内の他の機関の研究者と協力して、グラディエントフロー法を用いて非物理的な重いクォークに対する状態方程式を求めることに成功しており、今後もこの方法を用いた QCD 熱力学の研究を継続する予定である。次の目標は、物理点における 2+1 フレーバーQCD の状態方程式の決定である。また、CCS の研究者は格子 QCD コミュニティーの主要な挑戦的研究課題である温度と化学ポテンシャルをパラメータとする QCD の相構造の決定にも挑んでいる。この研究は、Wilson フェルミオンを用いることによって、クォーク質量が縮退した 3 フレーバーQCD から、2+1 フレーバーQCD および 4 フレーバーQCD(スタッガードクォークを用いた結果との比較によってユニバーサリティーを検証する)へと拡張されている。3 フレーバーQCD の研究では、臨界終点の温度を T_E= 134(3) MeV と決定することに成功している。

iv) Application of the Tensor Network scheme to Quantum Field Theories: The group has been investigating the application of the Tensor Network approach to features of quantum field theories, mainly in lower dimensional theories but also in the four-dimensional Ising model. This is a promising technique which avoids many of the generic problems in Monte-Carlo simulations, some numerical (very significant reduction of computational cost) but more importantly some theoretical (sign and complex action problems).

iv)テンソルネットワーク法の量子場の理論への応用: 本グループは、テンソルネットワーク法を用いて量子場の理論を解析することを試みており、これまで主に低次元の理論と 4 次元のイジングモデルの解析に成功している。テンソルネットワーク法は、モンテカルロ法に内在する多くの本質的問題を解決している有望な手法である。例えば、数値

的には、計算コストの劇的な削減を可能にし、より重要な点として、符号問題や複素作用問題などの理論的問題も解決している。

CCS members have developed the Grassmann version of the tensor renormalisation group algorithm, allowing them to deal with the Grassmann variables directly. Among several interesting studies has been the explicit demonstration of the Silver Blaze phenomenon in two-dimensional complex φ^4 theory, showing that the average phase factor in the Boltzman weight decreases quickly with the chemical potential. We note that the applications of the Tensor Network scheme features in the Future Plan subsection of the group's report, but no detail is given as to the physics which will be studied.

CCS の研究者はテンソル繰り込み群法の Grassmann 数版を開発し、Grassmann 変数を直接取り扱うことを可能にした。これまで様々な興味深い結果が得られているが、その中でも、2 次元複素 φ^4 理論の解析において、Boltzman ウェイトが化学ポテンシャルの増加とともに急速にゼロに近づくにもかかわらず、Siler Blzaze 現象の発現を実証したことは印象的である。評価用レポートの将来計画には、テンソルネットワーク法の量子場の理論への応用に関する記述があるが、対象とする具体的なモデルについては詳細が与えられていない。

v) Numerical study of conformal theories: Some popular models beyond the Standard Model are almost "conformal" in that the β-function is almost zero. It is believed that QCD-like theories for a range of N_f massless quark flavours have conformal symmetry. In this subsection, the group describes their numerical investigations between 2012-2017 of such theories finding, for example, that there exist conformal regions for $N_f = 7$, 8, 12 and 16 and confirmed that infrared fixed points exist in these theories. We note that there is no mention of continuing this research in the Division's future plans.

v)コンフォーマル理論の数値的研究: 標準理論を超えるモデルの候補として広く知られているものの中には、β 関数がほぼゼロになる、すなわち、近似的に"コンフォーマル"なものが存在する。例えば、質量を持たないクォークからなる仮想的な QCD を考え、そのフレーバー数がある一定の範囲の大きな数まで増加すると、コンフォーマル対称性を持つと信じられている。CCS の研究グループは、2012 年～2017 年の期間において、フレーバー数 N_f=7,8,12,16 においてコンフォーマル領域が存在することを発見し、これらの場合に赤外固定点が存在することを確認した。評価用レポートの将来計画には、本研究の継続可能性について触れられていない。

Summary. The commiteee congratulates the Division of Particles for its wide-ranging and interesting programme of research in Lattice Field Theory in the review period. We look forward to the research outlined in the future plan, in the three areas of the exploitation of the PAC10 configurations, QCD dynamics at finite temperature and density and in the application of the Tensor Network scheme. In order to gain an optimal scientific return for the huge investment in generating the PAC10 configurations, perhaps the group could encourage new collaborators with interests beyond that found among its CCS members and current collaborators.

まとめ 本評価委員会は、今回の評価期間において、素粒子物理研究部門によって幅広く且つ興味深い格子上の場の理論の研究プログラムが遂行されたことを称賛したい。評価用レポート中の将来計画には、PACS10(訳注：英文中の PAC10 は typo)配位を用いた

物理計算、有限温度・有限密度下における QCD ダイナミクスの研究、テンソルネットワークスキームの格子上の場の理論への応用、の 3 つの領域における研究計画が記載されており、今後の研究成果に期待している。PACS10(訳注：英文中の PAC10 は typo)配位の生成は野心的な試みであり、それから得られる科学的成果を最大化するためには、CCS 内の研究者あるいは現在の共同研究者に留まらず、新たな外部の共同研究者を獲得していくことが望まれる。

2.2 Division of Astrophysics
宇宙物理研究部門

Scientific Programs
The astrophysics group, led by Prof. Umemura, includes 7 faculty members, 8 postdocs, and 23 graduate and undergraduate students. With a total of 38 members, the group has reached critical mass and has undertaken a broad research program that spans many state of the art topics in astrophysics and numerical science. Furthermore, the work being done also involves several multidisciplinary projects in computational astrobiology and computational bioimaging, and extensive collaborations with other divisions at the Center for Computational Sciences.

研究プログラム
宇宙物理グループは、梅村教授によって率いられ、7 名の教員、8 名のポスドク、23 名の大学院生並びに学部生がいる。この合計 38 名のメンバーによって、大規模なグループとなっており、宇宙物理および計算科学の多くの最新研究トピックスをカバーする幅広い研究プログラムを実施している。さらに、計算宇宙生命、計算バイオイメージングなど、複数の学際的なプロジェクトを推進するだけでなく、CCS の他の部門との広範な共同研究も行ってきた。

One focus of the Umemura group has been to model the formation of supermassive black holes in the centers of galaxies. It is well-known that most, if not all galaxies harbor such black holes and energy released from them is a key element to the evolution of galaxies. The group has proposed a novel theory for the origin of these black holes in which repeated mergers of lower mass black holes in a gas-rich environment eventually result in a supermassive black hole with properties similar to those inferred from observations. This work was carried out using simulations that combine N-body dynamics with gas dynamical drag and the emission of gravitational waves.

梅村教授の研究グループの主要テーマの一つは、銀河中心の超巨大ブラックホール形成の理論モデル構築である。大部分の銀河は、そのようなブラックホールを持っており、そこで解放されるエネルギーが銀河進化に決定的な役割を果たしていることが良く知られている。梅村教授のグループは、このブラックホールの起源として、より小さなブラックホールが、ガスが豊富な環境で合体を繰り返し、最終的に観測されているような性質に至るという新しい理論を提唱している。この研究は、ガスの力学的摩擦を入れた N 体計算と重力波放出効果を結合したシミュレーションによって行われた。

The Yoshikawa group has done interesting research on the impact of massive neutrinos on the growth of large-scale structure. This work has been carried out with Vlasov simulations that treat neutrino free streaming accurately, which affects the growth rate of large-scale structure in a manner that depends on neutrino mass. Ongoing efforts to measure properties of the Universe to better than percent accuracy using cosmological surveys will rely critically on simulations of the type being carried out at the CCS to constrain neutrino masses.

吉川講師の研究グループは、有質量ニュートリノが大規模構造の成長に与える影響について興味深い研究を行っている。この研究は、ニュートリノ質量に依存し、大規模構造の成長率に影響を与えるニュートリノの無衝突流を正確に扱うブラソフ計算によって行われたものである。宇宙論的なサーベイによって、パーセント以上の精度で宇宙を測ろうという現在進行中の取り組みは、今後、CCS で行われているニュートリノ質量に制限を与えるこのタイプの計算に決定的に依存することになるであろう。

The Yajima group has performed cosmological simulations to examine the properties of forming galaxies during the epoch of reionization. Detailed radiative transfer calculations are then employed to predict fluxes from these forming galaxies in Lyman-alpha and at sub-millimeter wavelengths. The results can in turn be used to interpret observations made by ALMA and the upcoming JWST mission.

矢島准教授の研究グループは、宇宙再電離期に形成される銀河の性質を探究する宇宙論的なシミュレーションを行ってきた。それらの形成中の銀河から放射されるライマン α やサブミリ波の強度を予言するため、詳細な輻射輸送計算を行っている。これらの結果は、ALMA やもうすぐ始動する JWST ミッションによる観測の解釈に使うことが可能である。

The Wagner group is heavily engaged in work to simulate the impact of jet feedback from supermassive black holes in the interstellar medium of galaxies. It is believed that feedback of this type is vital for understanding how galaxies evolve and, in particular, how star formation is regulated and shut down in the most massive galaxies that become red and dead. Understanding of how jets interact with a multiphase medium is a key element in developing more physically motivated models for large-scale cosmological simulations of galaxy formation. The work being carried out by the Wagner group is state of the art and one of the few efforts to model jet interaction with a multiphase gas in detail.

Wagner 助教の研究グループは、超巨大ブラックホールからのジェットによる銀河の星間物質に対するフィードバックの影響についてのシミュレーションに専心している。このタイプのフィードバックは、銀河がどのように進化するか、特に大きな銀河において星形成がどのように抑制されて停止し、活動の無い赤い銀河となるかを理解する上で極めて重要である。ジェットが多相の星間物質とどのように相互作用するかは、銀河形成の大規模なシミュレーションにおいて、より物理的なモデルを構築するために、重要な要素である。Wagner 助教のグループによって行われてきた仕事は、最新鋭のものであり、多相ガスとジェットの相互作用を詳しくモデル化する数少ない仕事の一つである。

The Mori group has carried out simulations of low-mass galaxies to study the impact of feedback from supernovae on the structure of dark matter halos. Cosmological N-body simulations suggest that dark matter halos are generically cuspy, with rising power-law density profiles at the center. However, observations of satellite galaxies around the Milky Way indicate that the dark matter halos of these objects have flat central density profiles, contrary to expectations. The source of this discrepancy is unknown. One possibility is that the dark matter is collisional on small scales, which would represent a significant modification to the standard cold dark matter paradigm. Another cause may be feedback from supernovae acting in an episodic fashion, setting up oscillations that interact gravitationally with the dark matter in a resonant manner. The simulations and linear analysis done at the CCS show that this is a viable explanation for the non-cuspy profiles seen in local satellite galaxies.

森准教授の研究グループは、ダークマターハローの構造に対する超新星からのフィードバックの効果を調べるために、低質量銀河のシミュレーションを行ってきた。宇宙論的な N 体計算では、一般的にダークマターハローは、銀河中心での密度分布のベキが大きくなるというカスプをもつことが示唆されている。しかしながら、天の川銀河の周りの衛星銀河の観測は、予想に反して、中心の密度分布が平坦になっていることを示している。この不一致の要因は分かっていない。一つの可能性は、ダークマターが小スケールでは衝突するというものであり、これは標準的な冷たいダークマターパラダイムの大幅な変更を意味する。もう一つの可能性は、超新星からのフィードバックが周期的に起きて、ダークマターに重力的に共鳴するような振動を引き起こすというものである。CCS で行われてきたシミュレーションと線形解析は、局所衛星銀河に見られるカスプの無いダークマター密度分布の有力な説明となりうることを示している。

The Ohsuga group has performed MHD simulations in a general relativistic context to follow disk accretion flows around black holes and neutron stars. The calculations demonstrate that super-Eddington accretion in a non-spherical geometry produces power jets with velocities of order 0.3-0.5 the speed of light. Radiative transfer done in postprocessing indicate that the predicted x-ray spectra from super-Eddington accretion onto magnetized neutron stars are consistent with those measured for ultraluminous x-ray sources.

大須賀教授の研究グループは、ブラックホールや中性子星の周りの円盤ガス降着を調べるため、一般相対論的な枠組みで磁気流体力学シミュレーションを行ってきた。計算により、非球対称な超エディントン降着が、光速の 0.3-0.5 倍の強力なジェットを生み出すことが示されている。また、ポストプロセスで行われた輻射輸送計算により、磁化された中性子星への超エディントン降着から予言される X 線スペクトルは、観測されている超高光度 X 線源のスペクトルと整合することが示されている。

Inoue and collaborators have studied the dynamical stability of spiral arms in galaxies using a linear stability analysis. Observations suggest that high-redshift galaxies are clumpy and one explanation for this is that spiral arms under some conditions can fragment. The work carried out by Inoue and collaborators yields a dispersion relation for a thin spiral arm that predicts the conditions under which it may fragment and the resulting masses of the clumps, which can then be compared with observations.

井上研究員とその共同研究者は、線形安定性解析により、銀河の渦状腕の力学的安定性を調べてきた。観測で、高赤方偏移銀河が多くの塊からなっていることが示唆されており、その説明の一つは、渦状腕が何らかの条件の下で分裂する可能性である。井上研究

員と共同研究者による研究によって、細い渦状腕が分裂する条件と塊の質量を与える分散関係式が明らかになった。これは、今後観測と比較できるものである。

Development of algorithms
計算アルゴリズム開発

The astrophysics group has an impressive track record of developing and implementing novel algorithms on a wide range of computer architectures. Many of the codes are being used by researchers at other locations in Japan and in other countries.

宇宙物理グループは、幅広い計算機アーキテクチャの下で、新たなアルゴリズムを開発し実装してきた素晴らしい実績をもつ。計算コードの多くは、日本や海外の他機関の研究者にも使われている。

The SEURAT code is used to do mesh-free radiative transfer on hydrodynamical simulations carried out with smoothed particle hydrodynamics (SPH). The code is based on a Monte Carlo treatment in which ray tracing is done directly on SPH data.　The main application to date has been to Lyman-alpha radiative transfer, including scattering and absorption by dust. A variety of tests have been performed to validate the code. The adaptive nature of SEURAT makes it ideal for following the propagation of Lyman-alpha photons in the interstellar media of objects such as Lyman-alpha emitters (LAEs).

SEURAT コードは、SPH 法を用いて行われた流体計算に対して、メッシュを張らずに輻射輸送を計算するものである。このコードは、モンテカルロ法に基づいて、SPH データに対して直接レイトレーシング計算を行う。これまでの主たる応用は、ダストによる散乱や吸収を含めたライマン α 輻射輸送である。様々なテストを行い、コードの信頼性が立証されている。SEURAT コードの SPH への適合性は、ライマン α 輝線天体（LAEs）のような天体において、星間媒質中のライマン α 光子の伝播を追う上で理想的なものであるといえる。

The UWABAMI code solves the equations of magnetohydrodynamics in a general relativistic curved spacetime. The M1 closure method is used to follow the propagation of radiation fields as they interact with the matter field. The INAZUMA code follows the radiation field in a more precise manner by directly solving the equations of radiative transfer. This approach has been used to predict the emission from super-Eddingtion accretion flows around black holes and neutron stars. The RAIKOU code is a multi-frequency approach to calculating radiative transfer in a Kerr spacetime using a Monte Carlo scheme. This code is mainly used in postprocessing to generate observables and was used to analysis the recent observations of the supermassive black hole in M87 by the Event Horizon Telescope.

UWABAMI コードは、一般相対論的な曲率時空において磁気流体力学方程式を解くものである。物質場と相互作用する輻射場の伝播を追うために M1 クロージャー法が用いられている。INAZUMA コードは、輻射場をより正確に追うために、輻射輸送方程式を直接計算するものである。この方法は、ブラックホールや中性子星の周りの超エディントン降着流からの放射を予言するのに使われている。RAIKOU コードは、モンテカルロ法を使って、カー時空における輻射輸送を多振動数で計算するものである。このコード

は、観測と比較するためのポストプロセス計算で使われ、イベントホライズン望遠鏡で最近観測された M87 の超巨大ブラックホールの観測の解析にも使われた。

The ARGOT code is a parallel radiative transfer code that has been used especially to predict emission from high redshift galaxies. The code incorporates separate treatments of point sources and diffuse radiation fields from spatially extended sources. The algorithm makes impressive use of the various computing capabilities available on the Cygnus supercomputer. CPUs and GPUs are used for the point sources and the diffuse, extended sources are handled by FPGAs. These special purpose components have been shown to greatly enhance the performance of the code, in some cases by roughly an order of magnitude.

ARGOT コードは、並列版の輻射輸送コードであり、特に高赤方偏移銀河からの放射を予言するために使われてきた。このコードは、点光源と広がった光源からの拡散光を別々に取り扱っている。このアルゴリズムは、Cygnus スーパーコンピュータの多様な計算機能を見事に使いこなしている。点光源には CPU と GPU が使われ、拡散した広がった光源は FPGA で計算されている。これらの専用計算機部はコードの計算性能を大幅に向上することが示されており、ケタで向上している場合もある。

The TRINITY code has been developed to perform three dimensional, time-dependent radiative transfer calculations of near infrared radiation for applications in optical bioimaging and optical tomography. A variety of physical processes have been incorporated into TRINITY to allow it to handle multiple scattering events and high levels of absorption by, e.g., cancerous tumors in which blood is concentrated.

TRINITY コードは、光バイオイメージングと光断層撮影への適用を目指し、3 次元の時間依存輻射輸送計算を実行するために開発されてきた。TRINITY コードには、様々な物理過程が組み込まれており、例えば血液集中が起る癌腫瘍のような場所での多重散乱や強い吸収が扱えるようになっている。

Multidisciplinary and collaborative programs
学際的共同研究プログラム

The astrophysics group has been involved in numerous collaborations with other groups at the CCS. With the Division of High Performance Computing Systems, researchers aided in the codesign of computer architectures and algorithms to take advantage of hardware optimized for specific applications. This is one of the unique aspects of the CCS and the astrophysics group has been one of the main drivers behind the codesign strategy. This effort resulted in the ART and ARGOT codes for radiative transfer that make effective use of CPUs, GPUs, and FPGAs and has resulted in an approach that is significantly more efficient than would otherwise be possible.

宇宙物理グループは、CCS の他のグループと数多くの共同研究を行ってきた。高性能計算システム研究部門とは、特定のアプリケーションに特化したハードウェアの利点を引き出すために、計算機アーキテクチャやアルゴリズムのコデザインを進めてきた。これは、CCS のユニークな側面の一つであり、宇宙物理グループは、コデザイン戦略の主たる牽引者の一つとなってきた。この努力は、CPU, GPU, および FPGA を効果的に使用

する ART や ARGOT といった輻射輸送コードで結実しており、他の可能性と比べても、遥かに有効な方法論となっている。

The effort in computational astrobiology is particularly impressive and involves 55 members at 22 institutions across Japan. This work cuts across a broad range of fields including computational astrophysics, computational planetary science, and computer science. To date, the science topics that have been covered are the growth of dust grains in turbulent protoplanetary disks, the formation of interstellar molecules, and the possible role played by circularly polarized light in the homochirality of amino acids.

計算宇宙生命の取り組みは、特に素晴らしく、日本全体で 22 機関、55 名の参加者がいる。この取り組みは、計算宇宙物理学、計算惑星科学、計算機科学といった広い分野に渡っている。これまで、乱流的原始惑星系円盤におけるダスト粒子の成長、星間分子生成、アミノ酸のホモキラリティにつながるうる円偏光波の役割、といった研究トピックスが探究されてきた。

Amino acids can be either left- or right-handed, yet living organisms consists almost entirely of the left-handed variety. Various explanations for this have been proposed, including theories that involve weak nuclear interactions. The astrophysics group is studying the role of circularly polarized light in determining the chirality of amino acids by examining the impact of non-spherical dust grains in star-forming regions on emergent radiation fields. The radiative transfer calculations performed by the group show that circularly polarized emission can be produced at a level of 10-20%, depending on the sizes of the scattering dust particles.

アミノ酸には、左手型と右手型があるが、生命体はほとんど全て左手型だけからできている。これについては、様々な説明がなされており、原子核の弱い相互作用によるものであるという説もある。宇宙物理グループは、星形成領域での非球対称ダスト粒子が輻射場に及ぼす影響を調べ、アミノ酸の鏡像対称性を引き起こす円偏光波の役割を探究している。このグループが行った輻射輸送計算は、散乱ダスト粒子のサイズに依存して、10-20%の円偏光波が生成可能であることを示している。

Work by Furuya and collaborators has focused on the formation of molecules in interstellar space and whether or not these molecules contribute to protoplanetary disks. A particular topic of interests concerns nitrogen isotope fractionation and the ^{14}N / ^{15}N ratio. This ratio varies widely in observed systems from ~ 440 in the Sun, to ~ 100-200 in comets, and ~ 1000 in the cores of molecular clouds. Furuya and collaborators have used kinetic Monte Carlo simulations with a treatment of surface chemistry on dust grains to understand the observed ratios of ^{14}N / ^{15}N, and proposed a novel scenario to explain the observations that includes a combination of N_2 photodissociation and NH_3 ice formation.

古家助教と共同研究者は、星間空間における分子生成と、その分子が原始惑星系円盤に寄与したか否かを集中的に研究してきた。特に興味深いトッピクは、窒素同位体の分別と ^{14}N / ^{15}N 比である。この比は、太陽で~ 440、彗星で~ 100-200、分子雲コアで~ 1000 と、観測される系で大きくばらついている。古家氏と共同研究者は、観測されている ^{14}N / ^{15}N 比を理解するために、ダスト表面の化学反応を扱った動力学的モンテカルロ計算

を用い、N_2 分子の光解離と NH_3 氷の組み合わせで、観測を説明できる新たなシナリオを提唱している。

The Umemura group has performed simulations of dust coagulation in turbulent protoplanetary disks by solving the Navier-Stokes equations coupled with a treatment of dust particle coagulation. An important conclusion of this work is that turbulent clustering of dust can promote sticking, perhaps alleviating the problem of how micron sized dust particles can grow to the centimeter and larger bodies required for protoplanets to form.

梅村教授のグループは、ナビエストークス方程式を解いて、ダスト粒子の合体を取り扱い、乱流的原始惑星系円盤におけるダストの合体成長のシミュレーションを行ってきた。この仕事の重要な結論は、ダストの乱流的集中化がダストの付着を促進することであり、これによって、ミクロンサイズのダストが、どのようにして原始惑星形成に必要なセンチメートル、さらにそれ以上の大きさの塊に成長できるかという問題を解決しうるというということである。

The astrophysics division has also been involved in collaborations with researchers in the medical sciences related to optical bioimaging, with the eventual objective of implementing diagnostic procedures that are less invasive and with fewer side-effects than traditional methods based on magnetic resonance imaging or CAT scans. To this end, the group has performed radiative transfer calculations to study the propagation of near infrared light through human tissue to determine the feasibility of using this approach for optical tomography and bioimaging.

宇宙物理研究部門はさらに、MRI や CT スキャンに基づく従来の方法よりも侵襲性が小さく副作用の少ない診断法を実装することを最終目標として、光バイオイメージングに関する医学分野の研究者との共同研究に参加してきた。そして、宇宙グループは、この方法による光断層撮影やイメージングの実現性を示すべく、人体の組織中での近赤外光の伝播を調べる輻射輸送計算を実行してきた。

Strategic points
戦略的ポイント

The Division of Astrophysics is among the most productive groups at the CCS. The research covers applications in nearly all of the most important areas in modern astrophysics, from the formation of planets, to the formation of galaxies and large scale structure, the origin of supermassive black holes and gravitational radiation, and the origin of life in the Universe. This effort has been complemented by the development and implementation of a large number of computational algorithms that have significantly advanced progress in their scientific endeavors. Moreover, scientists in this group have been extremely engaged in the CCS and broader scientific community by establishing strong collaborations with other research groups at the University of Tsukuba and beyond. They have also been one of the main drivers in promoting the co-design philosophy that forms the basis for the CCS. The accomplishments of this group are well-represented by their long and impressive list of publications.

宇宙物理研究部門は、CCS の中で、最も生産性の高いグループの一つである。その研究は、惑星形成から、銀河・大規模構造形成、超巨大ブラックホールと重力波の起源、宇

宙おける生命起源まで、現代宇宙物理学の最も重要な領域の研究のほとんど全てをカバーしている。この取り組みは、彼らの尽力によって大きく発展した非常に多くの計算アルゴリズムの開発と実装の賜物である。さらに、このグループの研究者は、筑波大学や学外の組織との緊密な共同研究を確立することで、CCS 並びに広い科学コミュニティーと非常に深く関わってきた。彼らはまた、CCS の基盤となるコデザインの理念を推進する牽引者の一つとなってきた。このグループの実績は、膨大で素晴らしい業績リストに顕著に表れている。

In the future, efforts to develop ties with the international scientific community could enhance the visibility of the work being done by the Division of Astrophysics.　Gender diversity remains a serious issue for the division and, indeed, the CCS as a whole. Enhancing diversity should be a priority for the CCS in the coming years.

今後、国際的な研究コミュニティーとの密接な関係を増強することに注力すれば、宇宙物理研究部門で行われている研究の認知度は高まるであろう。性別多様性は、この部門でも CCS 全体でも、依然大きな問題である。今後何年かは、性別多様性を増すことを最優先課題とするべきであろう。

Planning for the development and implementation of future supercomputer platforms have been ongoing and it is expected that the Division of Astrophysics will continue to play a leading role in this effort. The possibility of taking advantage of the capabilities offered by the Fugaku supercomputer should be investigated.

これまで、次世代のスーパーコンピュータ技術の開発と実装の立案が行われてきたが、宇宙物理研究部門が、この取り組みの主導的役割を継続していくことを期待する。富岳スーパーコンピュータのもつ計算能力を活かす可能性も検討すべきであろう。

2.3 Division of Nuclear Physics 原子核物理研究部門

The Division of Nuclear Physics performs theoretical and computational research for nuclear quantum many-body systems. Their primary methods are based on the Energy-Density Functional theory, and various extensions thereof. These methods are used to investigate a range of important open questions in nuclear structure and reactions, such as nuclear fission and nuclear transmutation (both relevant for nuclear power plants), collective motion in nuclei, double-beta decay (which could open a window on physics beyond the Standard Model), as well as issues concerning the structure of neutron stars.

原子核物理研究部門では、原子核量子多体系に対する理論的かつ計算科学的研究が行われている。主な手法は、エネルギー密度汎関数理論と、その様々な拡張に基づいている。これらの方法を用いて、原子核構造や反応における種々の重要な未解決問題を研究している。具体的には、（原子力発電にも関連する）核分裂・核変換、原子核の集団運動、（標準模型を超えた物理に新たな道を開く可能性のある）二重ベータ崩壊、および中性子星の構造に関する課題等である。

In particular, the group has a long history in the development and application of Time-Dependent Density Functional Theory (TDDFT), not only in nuclear physics, but also in condensed matter physics. Indeed, Prof. Yabana, one of the developers of these methods, is affiliated with both the Division of Nuclear Physics and the Division of Quantum Condensed Matter Physics. Currently, he is the leader of the condensed matter group, but thanks to the unique structure of the CSS, he is also able to follow the ongoing research activities of the nuclear physics group.

特に、本部門は、原子核物理に限らず凝縮系物理においても、時間依存密度汎関数理論（TDDFT）の発展と応用に長年にわたり取り組んできた。実際、この方法の開発者の一人でもある矢花教授は、原子核物理部門と量子物性部門の両方に所属している。現在、矢花教授は物性グループのリーダーであるが、センターのユニークな組織構成を通じて、原子核物理研究部門で現在行われている活動にも十分関与できている。

Over the past six years, the nuclear physics group has developed several extensions to TDDFT. An improved Time-Dependent Hartree-Fock-Bogoliubov (HFB) approach has been developed and implemented numerically in order to elucidate the importance of pairing and deformation in medium and heavy nuclei. This method has successfully been applied to the description of nuclear fission in actinide nuclei (which is used as energy source in nuclear reactors) and to head-on collisions of superfluid nuclei. An important notion in nuclear structure is collective motion, which cannot be described in the naive application of TDDFT. The standard method is to use the Quasi-Random Phase Approximation (QRPA), however, this approach is computationally very demanding. The nuclear physics group has developed the Finite Amplitude Method, which is essentially an efficient iterative solution to the QRPA problem. This approach allows for calculations of, e.g., giant resonances; QRPA sum rules; massless Nambu-Goldstone modes associated with spontaneous symmetry breaking; and pairing rotation. A new development is the Adiabatic Self-consistent Collective Coordinate method (ASCC) to obtain optimal collective coordinates for describing collective motion. In combination with the Stationary Phase Approximation this is a promising new method to address a range of (weak) collective phenomena in nuclear physics.

過去６年の間に、原子核物理研究部門は、TDDFTの拡張にいくつも取り組んできた。改良された時間依存ハートレー・フォック・ボゴリューボフ（HFB）法を開発し、数値計算コードに実装することで、中重核における対相関と変形の重要性を明らかにした。この手法を用いて、アクチノイド領域核の核分裂（原子炉におけるエネルギー源）の記述に成功し、超流動原子核同士の正面衝突にも適用され成功を収めている。核構造の理解に重要な要素として集団運動が挙げられるが、TDDFTの単純な適用がうまく行かないことが多い。標準的な方法として準粒子乱雑位相近似（QRPA）が知られているが、この方法は多大な計算資源を必要とする。本部門では、有限振幅法を開発し、QRPA問題の高効率な反復解法を実現した。これによって、巨大共鳴、QRPA和則値、自発的対称性の破れに伴うゼロ質量の南部・ゴールドストーンモード、対回転などの解析が可能になった。また、断熱的自己無撞着集団座標法（ASCC）の新たな開発により、集団運動を記述する最適な集団座標を同定することができる。停留位相近似と組み合わせることで、この手法は、原子核物理における様々な集団現象（集団性の弱い現象も含む）の研究を可能にする新手法として大いに期待される。

Another topic is the calculation of nuclear matrix elements for neutrinoless double beta decay. Understanding the rates for this process, once observed, will be key to the discovery of physics beyond the Standard Model. Accurate knowledge of these matrix elements is essential to interpret current and future double beta decay experiments; current estimates of these nuclear matrix elements vary by a factor of three, which leads to an order of magnitude uncertainty in the decay rates. The group recently highlighted the importance of proton-neutron pairing for this decay.

もう一つの課題として、ニュートリノレス二重ベータ崩壊に関わる原子核行列要素の計算がある。もし観測されれば、標準模型を超えた物理の発見において、この崩壊率の理解が鍵となるであろう。行列要素を正確に知ることは、現在および将来における二重ベータ崩壊実験の解釈にとって非常に重要である。現状では、この行列要素の評価は計算によって３倍程度の違いがあり、崩壊確率に対しては１桁程度の不定性が残ってしまう。本部門の最近の研究により、この崩壊過程において陽子・中性子間の対相関が重要であることを明らかにした。

Since 2014 the group also participated in an ImPACT project (which aims at high-risk, high-impact R&D) “Reduction and Resource Recycling of High-level Radioactive Wastes through Nuclear Transmutation”. Traditionally, high-level radioactive waste is disposed of through vitrification in glass solid and burial in deep stable geological layers. The goal of this ImPACT program is to investigate nuclear reaction paths for long-lived fission products, and convert them into stable or short-lived nuclides; and ideally, convert a portion into re-usable rare metals. Within this collaborative project, the nuclear physics group at CCS is responsible for high-precision nuclear structure data necessary for the calculation of reaction cross sections. The group has performed DFT calculations for all nuclides up to the actinide region, and have created an open website, InPACS (Interactive Plot Atomic nuclei and Computed Shapes), that shows the calculated ground state shape, binding energy, densities, etc. This is a valuable resource for studying possibilities for nuclear transmutation and an excellent example of outreach to the general public about nuclear physics.

2014年以降、本部門は（ハイリスク・ハイインパクトのR&Dを目指した）ImPACTプロジェクト「核変換による高レベル放射性廃棄物の大幅な低減・資源化」に参加してきた。高レベル放射性廃棄物は、ガラス固化し地層深くに埋めて処分するというのが、これまで考えられてきた通常の方法であるが、このImPACTプログラムの目標は、長寿命核分裂生成物の核反応経路を究明し、それらを安定核種あるいは短寿命核種に変換、理想的には一部を再利用可能なレアメタルに変換する手法を探すことにある。この共同研究プロジェクトの中で、センターの原子核物理研究部門は、反応断面積計算に必要な高精度核構造データの提供を担当した。アクチノイド領域までの全ての核種に対してDFT計算を実行し、計算された基底状態の形状、束縛エネルギー、密度などを公開するオープン・ウェブサイトInPACS（Interactive Plot Atomic nuclei and Computed Shapes）を構築した。これは核変換の可能性を研究する貴重な資源であると同時に、原子核物理を一般大衆に向けに解説した素晴らしいアウトリーチの例となっている。

Another research topic is the structure of neutron stars. The structure of the inner-crust of a neutron star plays a crucial role in observed phenomena such as cooling of neutron stars and pulsar glitches. The nuclear physics group has very recently performed finite-temperature HFB calculations in three dimensions. Using shifted Krylov methods, these calculations are suitable for massively parallel computing. Preliminary results suggest a possible new phase of ‘nuclear pasta’ in the crust. Furthermore, gravitational waves provide information on the Equation of State inside the core neutron stars. The goal is to relate the gravitational waves to accurate microscopic description of nuclear matter. Models beyond the Standard Model could modify this relation: e.g., the presence of Dark Matter inside a neutron star can modify the gravitational waves from binary neutron star mergers.

その他の研究テーマとして中性子星の構造があげられる。中性子星の内殻（インナー・クラスト）の構造は、中性子星の冷却やパルサー・グリッチなど、観測現象において決定的に重要な役割を果たしている。原子核物理研究部門では３次元の有限温度HFB計算に最近成功したが、これは、シフト・クリロフ法を利用し、大規模並列計算にうまく適合させることで可能になった成果である。テスト計算段階ではあるが、クラストにおける原子核パスタの中に、これまで予想されていない新しい相を示唆する結果を得ている。また最近の研究では、中性子星コア内部の状態方程式の情報を重力波によって知ることができるようになり、重力波と核物質の微視的性質の間の関係を明らかにすることが重要な目標となっている。標準模型を超えたモデルがこの関係を変更する可能性もある。例えば、中性子星内部の暗黒物質の存在が、中性子星合体からの重力波に変更を加えるかもしれない。

In conclusion, the nuclear physics group has developed and applied various extensions of DFT to a number of interesting topics at the frontier of nuclear physics under the leadership of Prof. Nakatsukasa. Overall, the group has a good level of productivity with (on average) several publications per faculty member per year in high-quality refereed journals. Several of their former students and postdocs have continued their academic career, and are now (junior) faculty members; one postdoc (Dr. Wen) has received a ANPhA/AAPPS-DNP award for young scientist (2019), and two former students (Dr. Sekizawa and Dr. Ebata) have received a Young Scientist Award of the Physical Society of Japan. The group is well regarded worldwide, and has established collaborations with research groups domestically (RIKEN, U. of Tokyo, Niigata U., Kyoto U.) and worldwide (Warsaw University of Technology, Michigan State University, University of Jyvaskyla, Australian National University). They are successful in obtaining grant support, including support for international collaborations. Most of the research requires a significant amount of computing, and the group seems to have ample access to the necessary high-performance computing resources. They have developed their own numerical codes, which have a high parallel efficiency using hybrid MPI and OpenMP for parallelization; some of their codes are suitable to run on GPUs. The group clearly benefits from discussions with computer scientists in CCS, even though these interactions have not led to joint publications or truly joint projects.

結論として、原子核物理研究部門は、中務教授のリーダーシップのもと、DFTの様々な拡張を開発しそれを応用することで、原子核物理学のフロンティアにある興味深い課題を数多く研究してきた。質の高い査読ジャーナルに毎年教員一人当たり（平均として）数本の論文を出版しており、総体的に部門の生産性は良好なレベルにあるといえる。原子核物理研究部門の過去の学生やポスドクのうち数名は、アカデミックなキャリアを引き続き積むことで、現在は大学教員やそれに準ずる職についている。ポスドクの一人（Wen研究員）は若手研究者に対するANPhA/AAPPS-DNP賞（2019年）を受賞し、またグループに大学院生として在籍していた研究者（関澤、江幡）が日本物理学会の若手奨励賞を受賞している。本部門は世界的に注目を集める存在であり、国内外の研究グループ

と共同研究を確立している（国内：理研・東大・新潟大・京大、国外：ワルシャワ工科大学、ミシガン州立大学、ユバスキラ大学、オーストラリア国立大学)。また彼らは、国際共同研究への資金を含む、競争的資金の獲得に成功している。グループの研究の多くは大きな計算資源を必要としているが、十分な量のHPC資源へのアクセスを有していると思われる。MPIとOpenMPのハイブリッド並列によって高い並列効率をもつ計算コードは、彼ら自身によって開発されたものであり、その中のいくつかはGPU上での実行に適している。グループは明らかにセンター内の計算機科学者との議論から有益な助言を得ているが、連名での出版や真の共同プロジェクトにはまだ至っていない。

Moving forward, the group plans to continue their excellent work on collective motion in nuclei, nuclear reactions, and the physics of neutron stars. The committee encourages the Division to maintain collaborations with condensed matter physics through Prof. Yabana and to consider collaborating with the Division of Astrophysics on the physics of neutron stars. Furthermore, in two years one of the current faculty members (Prof. Hashimoto) reaches retirement age. That reduces the number of faculty members to essentially two (Prof. Nakatsukasa and Prof. Hinohara), since Prof. Yabana is focusing his research efforts almost exclusively towards condensed matter physics. The committee would therefore strongly recommend strengthening the Division of Nuclear Physics by hiring a new faculty member within the next two years, with an emphasis on computational nuclear physics in order to enhance interaction and collaborations with computer scientists in CCS.

将来に向けて、本部門では、原子核集団運動、核反応、中性子星の物理などに関する研究を高いレベルで継続する予定である。本委員会は、矢花を通した凝縮系物理グループとの共同研究を保持し、さらに中性子星の物理に関しては宇宙物理部門との連携を考慮することを推奨する。矢花教授の研究は凝縮系物理にほぼ集中しているため、2年後には、現在の教員のうち一人（橋本）が定年を迎え、グループの教員は実質的に2名（中務・日野原）となる。したがって、委員会は、今後2年の内に新たな教員メンバーを雇用することで原子核物理部門を強化し、センター内の計算機科学者との協力・共同研究を拡大することを強く推奨する。

2.4 Division of Quantum Condensed Matter Physics 量子物性研究部門

The research of the Division of Quantum Condensed Matter Physics address a wide range of method development pushing the boundaries on the modelling and simulation of complex dynamic processes away from equilibrium. These include the combination of Maxwell and TDDFT for light-matter interactions in molecular and large scales nanoparticles and solids, driven systems described by classical light-matter Hamiltonians, and simulations of time-resolved spectroscopies. Efforts include fundamental physics, algorithm development, and implementation and distribution through the SALMON software package. These efforts have a substantial intrinsic interest and are generating excitement among junior participants and the simulation community. This is an ambitious long-term investment on very challenging problems that takes advantage of the level of CCS resources and time scale. The output over the review period is in general excellent.

量子物性研究部門は、平衡から離れた複雑な動的過程のモデリングとシミュレーションの境界を押し広げる幅広い手法の開発に取り組んでいる。これらは、分子や大規模なナノ粒子や固体における光と物質の相互作用のためのマクスウェルと TDDFT の組み合わせ、古典的な光・物質ハミルトニアンで記述される系、および時間分解分光のシミュレーションを含む。この研究には、基礎物理学、アルゴリズム開発、そして SALMON ソフトウェアパッケージの実装と配布が含まれている。これらの研究は、それ自身に大きな関心が持たれており、若手研究者やシミュレーションコミュニティの中に刺激をもたらしている。これは、CCS の保有する高レベルで継続性のあるリソースを、非常に挑戦的な問題に対して投入する、長期に渡る野心的な投資である。レビュー期間中の成果は全般的に優れている。

During the breakout session, detailed presentations of the science conducted in the division by the postdocs and senior leader scientists were provided. Those presentations were very fruitful in helping the committee to understand the operation of the division and the science they were doing. The division addresses a remarkably broad spectrum of topics ranging from isolated atoms and semiconductor superlattices to bulk dielectrics and superconductors and strongly correlated material is covered in depth. The topics discussed included:

- Strong light-materials interaction in atoms, molecules and solids
- Nonlinear pump-probe spectroscopies and time-dependent density functional theory
- Photoinduced phenomena in strongly correlated electron systems
- Understanding the high Tc copper oxide superconductors and the proposal to use them as active elements in a quantum computer.
- Development of large-scale ab-initio software for computational materials design

Positive factors such as the high level of resourcing, the breadth of scientific and technical expertise across the institute. Many of their contributions are undoubtedly world-class.

分科会では、ポスドクとシニアな研究者により、部門内で進んでいる科学に関し詳細なプレゼンテーションが行われた。これらの発表は委員会にとって、部門の運営と彼らが行っている科学を理解する上で非常に有意義なものであった。この部門では、孤立原子や半導体超格子からバルク誘電体や超伝導体、強く相関した物質に至るまで、非常に幅広い分野のトピックを扱っており、深く掘り下げて取り扱われている。議論されたトピックは以下の通りである。

- 原子、分子、固体における強い光と物質の相互作用
- 非線形ポンププローブ分光と時間依存密度汎関数理論
- 強相関電子系の光誘起現象
- 銅酸化物高温超伝導体の理解と量子コンピュータの能動素子としての利用提案
- 計算材料設計のための大規模第一原理ソフトウェアの開発

高レベルなリソース、センター全体にわたる科学的・技術的な専門性の広がりなどがプラスの要因となっている。彼らの貢献は総じて、疑いなく世界レベルのものである。

Measures of success:

- **Top-level scientific publications** with large impact. They have published nearly hundred papers in the last 6 years (the complete list in pp. 98-107 of part-II document). This is an incredible production relative to the size of the division.
- **Code development** is one of flagships of the division. This division has a tradition of developing real-space DFT codes: RSDFT, RSPACE and SALMON. In 2011, the RSDFT

code originally developed in the division (Iwata and Oshiyama) received the Gordon-Bell Prize. At present SALMON is the project from the division that is most visible to the condensed matter and atomic physics communities.

- **High quality collaborations with experimental groups**. The members of this division have an excellent track record in keeping successful collaborations with top-experimental groups in the field at MPQ Munich (Germany), ETH Zurich (Switzerland), LBL at Berkeley (USA), University of Colorado Boulder (USA), Griffith Centre for Quantum Dynamics (Australia), Forcshungszentrum Jülich (Germany), Texas A & M University (USA) and TU-Wien (Austria)
- One measure of success of the division is the **attractive offers to senior scientists** from prestigious institutions. This is a good measure of the quality of science but also raises a warning about keeping a stable process to keep attracting the best young talents to the quantum condensed matter division of CCS.

成功の基準

- インパクトのある**トップレベル科学論文の発表**。過去 6 年間で 100 本近くの論文を発表している（part-II 文書の 98-107 ページに完全なリスト）。これは部門の規模に比べれば、非常に多くの成果である。
- **コード開発**はこの部門の最重要なものの一つである。この部門では、実空間 DFT コード、RSDFT、RSPACE、SALMON を開発してきた伝統がある。。2011 年には、当部門で開発した RSDFT コード（岩田・押山）が Gordon-Bell 賞を受賞した。現在 SALMON は、当部門のプロジェクトの中で、物性物理学や原子物理学の分野で最も注目されている。
- **実験グループとの質の高い共同研究**。当部門のメンバーは、MPQ ミュンヘン(ドイツ)、ETH チューリッヒ(スイス)、LBL バークレー(アメリカ)、コロラド大学ボルダー校(アメリカ)、グリフィス量子ダイナミクスセンター(オーストラリア)、ユーリッヒ研究センター(ドイツ)、Texas A&M 大学(アメリカ)、ウィーン工科大学(オーストリア)などのこの分野におけるトップレベルの実験グループとの共同研究を成功させてきた実績を持つ。
- この部門の成功の一つの指標は、名門機関から**部門のシニア研究者に対する魅力的なオファー**である。これは科学の質の高さを示す良い指標であると同時に、CCS の量子物性研究部門に若い優秀な人材を引き付け続けるための安定したプロセスを維持することの必要性を警鐘している。

Who are their competitors/peers? As for TDDFT activity the main competitors are the Theory Department at the Max Planck Institute for the Structure and Dynamics of Matter at Hamburg, where Dr. Sato is presently leading a group as a distinguished visiting scientist as part of his tenure track process at the University of Tsukuba and the one of Prof. Joachim Burgdorfer's group at TU-Wien. However, we can safely state that this competition is positive and synergetic, what is making the advances in the field of non-equilibrium physics advancing steadily. To a lesser extent, the groups in USA of John Rehr, Das Pemmaraju and Lin Wang are also direct competitors but in a very specific subfield of the research activities, namely the ones linked to core level spectroscopy.

競合相手は誰か？ TDDFT に関しての主な競合相手は、佐藤助教が筑波大学のテニュアトラックの一環として客員研究員として滞在しているハンブルクのマックスプランク

物質構造動力学研究所の理論部門と、ウィーン工科大学の Joachim Burgdorfer 教授のグループである。しかし、このような競争は、非平衡物理学の分野の進歩を着実に進展させる、前向きで相乗効果のあるものとなっている。米国の John Rehr、Das Pemmaraju、Lin Wang のグループも直接的な競争相手ではあるが、限られた分野、すなわちコアレベルの分光に関連した分野での競争である。

Research activities in the last 6 years by the different subgroups in the division

過去 6 年間に行われた、部門内の異なるサブグループによる研究活動

The committee finds that the excellent work done in the division in general, and in particular highlight the outcome of the groups of Prof. Yabana, Sato and Tong, that is excellent and can be considered, in any case, as worldwide reference. The division of quantum condensed matter physics has been highly successful in exploring forefront condensed matter and material science topics with state-of-the-art computational science tools. Development of highly parallelized codes for electronic structure calculations allowed ab-initio simulations of very complex systems and opened the door to realistic simulations of nanoscale electronic devices and light-field induced excited-states dynamics. One unique feature is the close interdisciplinary work with experiments. The highlights and main achievements in the last reporting period include:

委員会は、当部門で行われた研究は総じて優れており、特に矢花教授、佐藤助教、トン准教授のグループの成果が世界基準のものであり優れていると評価する。量子物性研究部門は、最先端の計算科学ツールを用いて、最先端の物性・物質科学のテーマを探求し、大きな成果を上げてきた。電子構造計算のための高度に並列化されたコードの開発により、非常に複雑な系に対する第一原理シミュレーションが可能となり、ナノスケールの電子デバイスや光により誘起された励起状態ダイナミクスに対する現実的なシミュレーションへの扉が開かれた。ユニークな特徴の一つは、実験との密接な協力である。最近の報告期間におけるハイライトと主な成果は以下の通りである。

- **Development of first-principles electron dynamics simulation code SALMON (**effort lead by Prof. Yabana together with many members of the division and other divisions). Yabana has been collaborating with Prof. Boku's group of Division of High-Performance Computing Systems on the code development and performance tuning of SALMON. He also joins meetings of Division of Nuclear Physics regularly where he is co-affiliated. There are many groups worldwide interested in these developments, in particular laser sciences with strong and ultrashort pulses, nano-optics (near field plasmonics) and ultrafast phenomena general and attosecond experimental groups in particular.

- 第一原理電子ダイナミクスシミュレーションコード **SALMON** の開発 (矢花教授が中心となり、当部門及び他部門の多くのメンバーとの協力による) 矢花教授は、高性能計算システム研究部門の朴教授のグループと協力して、SALMON のコード開発とパフォーマンスチューニングを行った。彼はまた、兼任する原子核物理研究部門のミーティングにも定期的に参加している。世界中の多くの研究グループがこれらの開発、特に、高強度・超短パルスを用いたレーザー科学、ナノオプティクス（近接場、プラズモニクス）、超高速現象全般と特にアト秒実験グループが、これらの開発に興味を持っている。

- **Theoretical Description of Pump-Probe Spectroscopies in Solids and Ultrafast dynamics in solids and 2D systems under strong laser field within TDDFT** (Prof. Yabana and Assistant Prof. Sato). The activities in this topic over the last five years has been quite productive and developed a number of directions beyond what was presented in the previous report, writing a number of excellent papers on light-enhanced electronics coupling, attosecond dynamics in solids, description of strong nonlinear phenomena as high harmonic generation and the characterization of exotic Floquet electronic structure in driven systems, and light-matter coupling effects in cavities. The experimental-theoretical collaborations are strong, with several articles co-authored with top experimental groups worldwide in the ultrafast dynamics of interacting electronic systems. The presentations given by the five postdocs (Dr. Hashmi, Dr. Yamada, Dr. Takeuchi, Dr. Noda and Dr. Yamada) have been compiling and presented exciting novel science and ideas done with the SALMON project.

- **TDDFT に基づく、固体中のポンププローブ分光、および高強度レーザー場下での固体および二次元系の超高速ダイナミクスに対する理論的記述**（矢花教授、佐藤助教)。この 5 年間のこのトピックに関する活動は非常に充実しており、光増強電子結合、固体中のアト秒ダイナミクス、高調波発生などの強い非線形現象の記述、駆動系におけるエキゾチックなフロケ電子構造の探究、キャビティ中の光物質結合効果など、前回報告された内容を超えて多くの方向に展開し、優れた論文が執筆されてきた。また、実験と理論の共同研究も強力に行われ、相互作用する電子系の超高速ダイナミクスに関しては、いくつかの世界のトップレベルの実験グループとの共著論文がある。ポスドク 5 名（Hashmi 博士、山田博士、竹内博士、野田博士、山田博士）の発表は、SALMON プロジェクトで行われている活発で新奇な科学とアイデアを含むものであった。

- **Attosecond dynamics in atoms and small molecules** (Ass. Prof. Tong). He works in the AMO (Atoms, Molecules, and Optics) field where he has developed his own efficient computer code for solving time-dependent Schrödinger equation in 2D and 3D geometries. He is also working in explaining those phenomena within TDDFT what opens a direct internal link to the group of Yabana. Highly evaluated in the field. Collaborating with many high-reputation experimental groups worldwide on forefront ultrafast phenomena in atoms and molecules

- **原子・小分子におけるアト秒ダイナミクス**（Tong 准教授）。Tong 准教授は AMO(Atoms, Molecules, and Optics)の分野で研究を行っており、2 次元および 3 次元形状において時間依存シュレーディンガー方程式を解くための効率的な計算コードを独自に開発している。また Tong 准教授は、TDDFT でこれらの現象を説明することにも取り組んでおり、矢花教授グループと関係している。この分野での評価は高い。高く評価されている世界中の多くの実験グループと協力して、原子・分子の超高速現象に関し最前線の研究を行っている。

- **Modelling the photoinduced electronic dynamics of strongly correlated materials using a simple Hubbard model Hamiltonian** (Lecturer Maeshima). He has reported his recent results on describing the optical responses of correlated material using Hubbard model and the generation on coherent phonon by a pulsed light. The work on light-matter interactions in solids and nanosized systems is solid, but the outcome is so far not high and with not much impact.

- 強相関物質の光誘起電子ダイナミクスに対する単純化したハバードモデルハミルトニアンを用いたモデリング（前島講師)。前島講師は、ハバードモデルを用いた強相関物質の光応答の記述と、パルス光によるコヒーレントフォノン上の生成に関する最近の成果を報告した。固体やナノサイズ系の光物質相互作用に関する研究は堅実だが、成果は今のところ高くなく、インパクトに乏しい。

- **Strongly correlated systems and superconductivity** (Ass.Prof. Koizumi). He has been working over that last ten years in the development of a method to calculate the Berry connection and current produced by it in a model for a high Tc cuprate superconductors. He is also proposing to use those superconductors as active elements for next generation quantum computers. The work seems interesting but is difficult to grasp and it is not having a marginal impact in the scientific community. The usefulness of those ideas is unclear. Still the research performed is sound and novel.

- 強相関系と超伝導（小泉准教授)。小泉准教授は過去 10 年間にわたり、銅酸化物高温超伝導体に対するモデルにおいて、ベリー結合とそれによって生じる電流を計算する方法の開発に取り組んできた。また、これらの超伝導体を次世代の量子コンピュータの能動素子として利用することも提案している。この研究は興味深いが把握することは困難であり、科学コミュニティにおけるインパクトは限られている。これらのアイデアの有用性ははっきりしない。しかしながら、行われている研究は（科学的に）適正であり新奇性がある。

Structure and personal of the division

部門の構成と人員

The quantum condensed matter division consist of 3 senior people (the deputy director of the institute, Prof. Yabana, and Associate Professors Tong and Koizumi) and three juniors, but one of them, Dr. Ono has taken a full professor position at Kobe University (he remains affiliated to the center as visiting professor). This staff is supported by six post-docs, five are working with Prof. Yabana on developing SALMON and the other one was working with Prof. Ono but will join the SALMON project from next April. SALMON is the largest and most visible project of the high-performance software activity of the division (towards massive exascale applications).

量子物性研究部門は、3 名のシニア（副センター長の矢花教授、Tong 准教授、小泉准教授）と 3 名の若手で構成されているが、そのうちの 1 名の小野准教授は神戸大学の教授に就任した（客員教授としてセンターに所属している)。これらのスタッフは、6 名のポスドクに支えられており、5 人は矢花教授と共に SALMON の開発に携わり、1 人は小野教授と共に研究をしていたが、今年 4 月から SALMON プロジェクトに参加する。SALMON は、当部門の高性能ソフトウェア活動（大規模エクサスケールアプリケーションに向けた）の中で、最大かつ最も目に見えるプロジェクトである。

In spite of the scientific success of the division, as reported above, we have identified an important issue linked to the age distribution of the permanent researchers in the division. All senior people are well above fifty and there is a **clear need to hire new younger professors that can keep the successful path set by the leader of the division, Prof. Yabana**. In this context, the incorporation of Dr. Sato as an International Tenure-Truck Professor, is a major step in that direction and has clearly strengthened the division, both in the scientific impact of the division as well as opening new international collaborations and collaborative projects. The committee recommends further strengthening the division by adding a couple of new tenure track positions for young researchers (young rising star in the field of computational condensed matter physics).

当部門の科学的な成功にもかかわらず、上述のように、当部門の常勤研究者の年齢分布に関わる重要な問題が見られる。部門のすべてのシニア研究者は 50 歳を超えており、**部門のリーダーである矢花教授がもたらした成功の道筋を維持できる若手教員を新たに採用する必要があることは明らかである。**この観点において、佐藤博士を国際テニュアトラック助教として迎え入れたことは、その方向への大きな一歩であり、部門の科学的なインパクトだけでなく、新たな国際共同研究や共同プロジェクトの開拓という点でも、明らかに部門の強化をもたらしている。委員会は、若手研究者（計算物性物理学分野の期待の星）を対象としたテニュアトラックの複数のポストを加えることで、当部門をさらに強化することを推奨する。

International Collaborations

A very active and fruitful network of experimental and theoretical collaborators has been successfully established over the years. This collaborative network has not only been reinforced since the last report in 2014 but increased. This conclusion is supported by the large set of joint publications in top-level journals with those groups and the relatively large number of citations they have received in this short period of time.

国際的な協力

非常に活発で実りある実験・理論共同研究者のネットワークが、長年にわたって成功裏に構築されてきた。この共同研究ネットワークは、2014 年の前回の報告書以降、強化されただけでなく、増加している。この結論は、これらのグループとの共同出版物がトップレベルの学術誌に多数出版されていることや、短い期間での比較的多くの被引用数によって裏付けられている。

2.5 Division of Life Sciences 生命科学研究部門

2.5.1 Biological Function and Information Group 生命機能情報分野

The Biological function and Information group is highly active in several research areas:

生命機能情報グループは様々な研究領域において、極めて活発に研究を行なっている。

i) **QM/MM studies of enzymatic reactions.** The unique three-dimensional structures of enzymes and their dynamics are tailor made to catalyze specific chemical reactions with high efficiency. However, since enzymes are complex protein molecules with thousands of atoms and have complicated structures that are dynamic, it is very hard to pin down and understand the underlying microscopic mechanism at atomic levels. In addition, enzyme reactions are inherently quantum mechanical and require quantum mechanical treatment. All these features combined make it extremely difficult, if not impossible, to truly understand how enzyme works in theory. The group has adopted the state-of-the-art QM/MM approach, in which the active center of the enzyme where the reaction occurs is modeled by quantum mechanics while the rest of the enzyme is treated by classical molecular dynamics. However, the QM/MM simulation of an enzyme reaction requires significant computational resources as well as computational strategies in order to be successful and obtain physically meaningful results. Prof. Shigeta is a world class leader in developing and applying QM/MM methods to study practical enzyme reaction systems to elucidate the reaction mechanisms. Prof. Shigeta and his group members have carried out extensive QM/MM studies for a range of important protein systems, including the important photosystem II (PS II) to investigate the formation mechanism of O_2 in the oxygen evolving complex; redox reaction of bilirubin oxidase; the hydration of nitriles in nitrile hydratase. The group is very active in this research area and many of these works are state-of-the-art in the field.

i) **QM/MM** による酵素反応の研究

酵素は、独自の３次元構造とそのダイナミクスにより、特定の化学反応を高効率に触媒するように作られている。しかし、酵素は数千個の原子からなる複雑なタンパク質分子であり、複雑で動的な構造を持っているため、原子レベルでの微視的なメカニズムを解明することは非常に困難である。 また、酵素反応は本質的に量子力学的な現象であり、その計算には量子力学的な取り扱いを必要とする。これらすべての特徴が組み合わさって、酵素の仕組みを理論的に理解することは、不可能ではないにしても、極めて困難といえる。当グループでは、反応が起こる酵素の活性中心を量子力学的にモデル化し、それ以外の部分を古典分子動力学的に扱うという、最先端の QM/MM アプローチを採用している。しかし、酵素反応の QM/MM シミュレーションを成功させ、物理的に意味のある結果を得るためには、膨大な計算資源と計算戦略が必要となる。重田教授は、実用的な酵素反応系の研究に QM/MM 法を適用して反応機構を解明する世界的なリーダーの一人といえる。特に重田教授のグループは、重要な光化学系 II（PS II）の酸素発生複合体における酸素の生成機構の解明、ビリルビン酸化酵素の酸化還元反応、ニトリルヒドラターゼにおけるニトリルの水和反応など、様々な重要なタンパク質系を対象とした QM/MM 法による研究を行ってきた。 当グループでは、この分野の研究に非常に積極的に取り組んでおり、その多くはこの分野の最先端の研究成果といえる。

ii) **Development of enhanced sampling method.** The study conformational transition of proteins is essential to understanding the function of proteins. Common molecular dynamics (MD) simulations typically sample only local structures of proteins. The Shigeta group proposed a relatively simple enhanced sampling method to study conformational transitions of proteins. The method consists of starting with different initial structures and runs many short time dynamics to select those trajectories that have good transitions to desired new conformations, and the process is iterated until convergence. This method is relatively simple to use and effective for some protein systems.

ii) サンプリング方法の改良

タンパク質の機能を理解するためには、タンパク質の構造変化の研究が不可欠である。従来の分子動力学（MD）シミュレーションを用いた研究では、タンパク質の局所構造のみをサンプリングするのが一般的である。一方、重田教授グループは、タンパク質の構造変化を研究するための比較的簡単なサンプリング法を提案した。この方法は、異なる初期構造から出発し、多くの短時間ダイナミクスを実行して、目的の新しい構造への遷移が良好な軌道を選択し、収束するまで繰り返し実行するというアルゴリズムに基づいている。この方法は比較的簡単に使用でき、一部のタンパク質システムに有効である。

iii) **Astrobiology.** The Shigeta group also carried out research to investigate the glycine formation in extraterrestrial environments. These studies are based on quantum chemistry, i.e., DFT method to calculate barriers to various related reactions. Their result supports the hypothesis that the radical process is the most likely process for glycine formation. This is of interest to the research on the origin of life in universe. The astrobiology studies have been performed with collaborations with the Divisions of Astrophysics and Quantum Condensed Matters Physics. Five papers are already published.

iii) アストロバイオロジー

重田教授グループでは、地球外環境でのグリシン生成を調べる研究も行っている。これらの研究は、DFT 法などの量子化学計算に基づいて、様々な関連反応の障壁を計算している。その結果、ラジカル反応がグリシン生成の最も可能性の高いプロセスであるという仮説を支持している。このことは、宇宙における生命の起源の研究においても興味深い。アストロバイオロジーの研究は、宇宙物理学部門と量子物性物理学部門との共同研究体制の元で行われており、すでに 5 本の論文が発表されている。

iv) **Computational biomolecular medicine.** The group employed its own method, the parallel cascade selection MD (PaCS-MD), to investigate the permeation of the cell membrane (modeled by POPC lipid bilayer) by cyclic peptides. The main purpose is to simulate how peptides penetrate cell membranes. This should be of interest to researchers developing peptide drugs.

iv) 計算生体分子医科学

当グループでは、独自の手法である並列カスケード選択型 MD（PaCS-MD）を用いて、環状ペプチドによる細胞膜（POPC 脂質二重層でモデル化されたもの）への浸透を調べている。主な目的は、ペプチドがどのように細胞膜を透過するかを再現することで、ペプチド医薬品を開発している研究者にとって興味のある成果と考えられる。

v) **Photosynthetic system.** The group also used Marcus electron transfer theory coupled with the fragment molecular orbital (FMO) approach to study the photosynthetic system and the aromaticity of photoexcited molecules.

v)　　光合成系の研究

　フラグメント分子軌道（FMO）アプローチとマーカス電子移動理論を併用して、光合成系と光励起分子の芳香族性を研究している。

vi)　　The Shigeta group also performed first principle analysis of ammonia adsorption and desorption on GaN surface as well as first-principles calculations of Na ion containing transition metal oxides. These studies are mainly based on a quantum chemistry approach using the DFT method. These studies are closely related to possible new materials applications such as new battery technology.

vi)　　重田教授グループはまた、GaN 表面におけるアンモニアの吸着・脱着の第一原理解析と Na イオン含有遷移金属酸化物の第一原理計算を行った。これらの研究は、主に DFT 法を用いた量子化学的アプローチに基づいており、新しい電池技術などの新材料応用の可能性と密接に関連している。

vii)　　**Development of GPU-accelerated software.** Another important push by the Shigeta group is to develop software for efficient computational application, particularly, on GPU machines. This effort is technically challenging and labor intensive. They are working on three specific software based on the fragment molecular orbital (FMO), DFTB and Car-Parrinello Molecular Dynamics (CPMD) methods for acceleration of MD and QM calculations. This project is carried out in close collaboration with members of the Division of High-Performance Computing System (HPCS). Good progress is already made in the FMO software for GPU acceleration with two published papers and one book chapter.

vii)　　**GPU を利用したソフトウェアの開発**

　重田教授グループのもう一つの重要な研究推進事項は、特に GPU マシン上で効率的に計算を行うためのソフトウェアを開発することである。この取り組みは技術的に挑戦的であり、多大な労力を要する。重田教授グループでは、フラグメント分子軌道(FMO)、DFTB、Car-Parrinello 分子動力学法(CPMD)に基づいた 3 つのソフトウェアを開発し、MD や QM の計算を加速している。このプロジェクトは、高性能計算機システム部門(HPCS)のメンバーと密接に協力して実施されており、GPU 加速した FMO ソフトウェアについては、すでに 2 つの論文と 1 つの本の章が出版されており、良好な進展が見られている。

Summary

In summary, the Biological Function and Information group led by Prof. Shigeta is highly research active and extremely productive and has made significant advances in several important research areas. Their research covers a relatively wide range of topics in the interface of physics, chemistry, biology, material and high-performance computing. The main theoretical tools they use are quantum chemistry, molecular dynamics and statistical mechanics. The group's research is carried out with extensive collaborations with many of their colleagues in other divisions, including the

Division of High Performance Computing System, the Division of Astrophysics, Computational Medical Sciences and also with external collaborators at the Institute for Space and Astronautical Sciences (ISAS) and Japan Aerospace Exploration Agency (JAXA), etc. It is fair to say that very few groups in the world have such extensive interdisciplinary research activity and expertise. The group has one of the most impressive track records in publications, with 128 publications (many of them in high impact journals), 7 conference proceedings, 9 book chapters and 2 patents, plus many awards. In light of the diverse research interests and directions, the committee feels that the group could put some effort to realign some of the research directions with more focus on those areas that the group has unique strengths.

概要

重田教授を中心とした生命機能情報グループは、非常に活発な研究活動を行っており、極めて生産性が高く、幾つもの重要な研究分野で大きな進歩を遂げてきた。彼らの研究は、物理学、化学、生物学、材料学、高性能コンピューティングなどの分野において、比較的幅広いテーマをカバーしている。主に量子化学、分子動力学、統計力学を用いて研究を行っている。また、このグループの研究は、高性能計算機システム部門、宇宙物理学部門、計算医科学部門、宇宙科学研究所（ISAS）、宇宙航空研究開発機構（JAXA）などの外部研究者との共同研究など、他部門の多くの研究者との広範な共同研究によって行われている。このような学際的な研究活動と専門性を持つグループは、世界でも非常に少ないと言ってよい。当グループは、128 の出版物（その多くはインパクトのある雑誌に掲載）、7 つの会議録、9 つの本の章、2 つの特許に加え、多くの賞を授与されており、出版物の実績は世界でも有数のものである。一方で、多様な研究の関心と方向性を鑑みると、委員会は、グループが独自の強みを持つ分野に焦点を当てて、研究の方向性を再調整した方が良いのではないかと感じている。

2.5.2 Molecular Evolution Group

分子進化分野

The Molecular Evolution Group, headed by Prof. Inagaki (group leader) with Ishitani (researcher), although rather small, is highly research active and productive. The group's research mainly focuses on the evolutionary process to understand the extant molecular mechanisms and genomes in microbial eukaryotic cells. The major works and accomplishments are stated below:

分子進化グループは、研究員である石谷博士と共に稲垣教授（グループリーダー）が中心となり、少人数ながら非常に活発な研究活動を行っている。 当グループでは、微生物の真核細胞に現存する分子機構やゲノムを理解するための進化過程を中心に研究を行っている。主な研究成果は以下の通りである。

i) **Global eukaryotic phylogeny.** The Inagaki group has made significant new progresses. Two specific examples follow. First, the group proposed a new super-group of eukaryotes and performed phylogenetic analyses based on a super-matrix including 97,002 amino acid positions in total. They recovered a robustly supported clade comprising collodictyonids, Rigifila, and

Mantamonas. Their study, an international joint research effort among groups in the US, Canada, and Japan, suggests that collodictyonids, Rigifila, and Mantamonas form a major eukaryote clade that has been overlooked in earlier studies. The work was published in Genome *Biol. Evol.* in 2018 and has been well cited. Second, highly modified mitochondrion-related organelles (MROs) exist in many anaerobic microbial parasites. The group examined the phylogenetic relationship among metamonads based on a super-matrix containing 159 proteins. The group analyzed super-matrix and also the transcriptomic data to resolve the relationship among the members of Metamonada and to predict proteins localized in the MRO for each metamonad species. By doing so, they successfully uncovered a complex history of ATP production machinery in diplomonads and dysnectes, and a correlation between the glycine cleavage machinery and lifestyles. Again, this is an internationally collaborative work involving groups in the US, Sweden, Czech Republic, Japan, and Canada, and the published work is well recognized and cited.

i) **真核生物大系統** 稲垣教授グループの研究には、大きな進捗があった。以下に 2 つの研究を挙げる。第 1 に合計 97,002 アミノ酸座位から構成される配列データセットによる系統解析を行い、真核生物の新しいスーパーグループを提案した。その解析では強いサポートのもとコロディクチオン類、Rigifila、Mantamonas からなる単系統群を復元した。この研究は、米国、カナダ、日本のグループによる国際共同研究であり、これまでの研究では見落とされていたコロディクチオン類、Rigifila、Mantamonas から構成される主要系統群が存在することを示唆している。本研究結果はGenome Biol. Evol誌に.2018年に発表され、多くの論文で引用数もされている。第 2 の研究は、多くの嫌気性微生物寄生虫に存在する高度に縮退したミトコンドリア関連オルガネラ（MRO）に関するものである。この研究では、159 タンパク質から構成される配列データを基にメタモナス類の系統関係を調べた。研究グループは、スーパーマトリックスとトランスクリプトームデータを解析することで、メタモナス類の種間関係を解明し、各メタモナス種の MRO に局在するタンパク質を予測した。これらの解析により、ディプロモナスや Dysnectes の ATP 生産機構の複雑な進化と、グリシン切断機構と生活様式（自由生活性と寄生性）との相関関係を明らかにすることに成功した。この研究は米国、スウェーデン、チェコ、日本、カナダのグループが参加した国際的な共同研究であり、その成果は高い評価うけ、他の論文に引用されている。

ii) **Evolution of mitochondria.** Due to the bacterial ancestry of mitochondria, most eukaryotes retain their own mitochondrial genomes. But the gene contents have been modified drastically during the evolution of eukaryotes. Finding optimal trees relating the sequences is computationally challenging with the increase in the number of species and genes. The Inagaki group sequenced and published the mitochondrial genomes of five eukaryotes belonging to Haptista (Chrysochromulina sp. and Marphrys sp.) and Cryptista (Palpitomonas bilix, Leucocryptos marina, and Hemiarma marina). They also sequenced and published mitochondrial genomes of two haptists and three cryptists Cryptophytes. These works are published in Mobile Genet Elements (2014 4:e29384), Sci Rep (2019 9:4850), and Genome Biol Evol (2016 8:3090–3098).

ii) **ミトコンドリア進化**ミトコンドリアの祖先は細菌であるため、ほとんどの真核生物

がもつミトコンドリアは独自のゲノムを保持しているが、ゲノムに含まれる遺伝子の種類は真核生物進化の過程で大きく変化している。生物種や遺伝子数が増加するため、配列データを基に最尤系統樹を見つけることは計算量的に困難である。稲垣教授グループは、ハプチスタ生物群（Chrysochromulina sp.と Marphrys sp.）とクリプチスタ生物（Palpitomonas bilix, Leucocryptos marina, Hemiarma marina）に属する合計 5 種の真核生物のミトコンドリアゲノムの配列を決定し、公開した。また、2 つのハプティストと 3 つのクリプティスト Cryptophytes のミトコンドリアゲノムを配列決定し、公開した。これらの論文は、Mobile Genet Elements（2014 4:e29384）、Sci Rep（2019 9:4850）、Genome Biol Evol（2016 8:3090-3098）に掲載されている。

iii) Evolution of plastids. The genomes of secondary non-photosynthetic plastids tend to be more reduced than those of photosynthetic plastids in terms of both genome size and gene repertory. The Inagaki group sequenced and analyzed the plastid genomes of non-photosynthetic species in two algal groups in order to retrace the reductive process (Tanifuji et al. 2020 Genome Biol Evol in press; Kamikawa et al. 2015 Mol Biol Evol 7:1133-1140). They revealed that distinct sets of photosynthesis-related genes were lost from the plastid genomes of multiple cryptophytes that lost photosynthesis separately. These works are performed in collaboration with Dr. Goro Tanifuji in National Museum of Nature and Science, Japan, and Dr. Ryoma Kamikawa in Kyoto University, Japan.

iii) **色素体進化** 二次的な非光合成種の色素体（葉緑体）のゲノムは、ゲノムサイズ、遺伝子レパートリーともに光合成種の色素体よりも縮退している傾向がある。稲垣グループは、この縮退過程を辿るために、2 つの藻類群の非光合成種の色素体ゲノムを配列決定し、解析した（Tanifuji et al. 2020 Genome Biol Evol in press; Kamikawa et al. 2015 Mol Biol Evol 7:1133-1140）。彼らは、光合成を別々に失った複数のクリプト藻の色素体ゲノムから、光合成に関連する遺伝子の異なるセットが失われていることを明らかにした。これらの研究は、国立科学博物館の谷藤吾朗博士、京都大学の神川龍馬博士との共同研究である。

The group sequenced the plastid genome of Lepidodinium possessing a green-colored plastid containing chlorophylls a and b and prepared a super-matrix containing 52 proteins that are encoded in the plastid genome. The work concluded that the ancestral Lepidodinium engulfed an alga belonging to Pedinophyceae, followed by the transformation of the endosymbiont alga into the current green-colored plastid. These results were published in Genome Biol Evol (2015 7:1133-1140). They also identified two dinoflagellate strains with green-colored plastids (TRD-132 and MRD-151; Sarai et al. Proc Nat Acad Sci USA 2020 in press) in collaboration with Drs. Takahashi and Iwataki at The University of Tokyo.

研究グループは、クロロフィル a と b を含む緑色の色素体を持つ Lepidodinium の色素体ゲノムの塩基配列を決定し、そのゲノムにコードされる 52 種類のタンパク質を含む系統解析用配列データを作成した。この系統解析により、Lepidodinium の祖先細胞がペ

ディノ藻類に属する緑藻を細胞内に取り込み、その共生緑藻が現在の緑色色素体となった結論づけた。この研究成果は、Genome Biol Evol（2015 7:1133-1140）に掲載された。また、東京大学の高橋博士および岩滝博士との共同研究で、緑色色素体をもつ 2 種類の渦鞭毛藻 TRD-132 株と MRD-151 株を発見した（Sarai et al. Proc Nat Acad Sci USA 2020 in press）。

iv) Evolution of bacterial endosymbionts in diverse eukaryotic cells. Some key events in the origin and diversification of eukaryotic cells involve the evolution of mitochondria and plastids from bacterial endosymbionts. Studying eukaryotic cells with recently evolved obligate endosymbiotic bacteria provides important insight into the transformation of endosymbionts into organelles. By sequencing and analyzing the first and second complete genome sequences of spheroid bodies in two rhopalodiacean diatoms Epithemia turgida and Rhopalodia gibberula, the Inagaki group proposed that the diatom-spheroid body endosymbiosis is a unique system for investigating the processes underlying the integration of a bacterial endosymbiont into eukaryotic cells. The works were published in Proc Nat Acad Sci USA (2014 111:11407-11412) and Sci rep (2017 7:13075). The group also investigated the origin and function of diverse bacterial symbionts in/associated with eukaryotes. The work was published in the prestigious journal, *Proc Nat Acad Sci USA* (2019 116:15973-15978).

iv) **各種真核生物がもつ共生細菌の進化** 真核細胞の起源と多様化のキーとなった重要な出来事のいくつかは、細胞内共生した細菌がミトコンドリアと色素体に進化したことと関連している。進化的に最近獲得された宿主細胞に依存した細胞内共生細菌をもつ真核生物を研究することで、細胞内内共生細菌からオルガネラへの進化についての重要な知見を得ることができる。稲垣グループは、2 種類の珪藻 Epithemia turgida と Rhopalodia gibberula の細胞内に共生する細菌（楕円体）の完全ゲノム配列を解析し、珪藻－楕円体間の共生関係は、細菌共生体が宿主である真核細胞に統合される過程を研究するためのユニークなシステムであることを提案した。これらの研究結果は、Proc Nat Acad Sci USA（2014 111:11407-11412）および Sci Rep（2017 7:13075）に掲載された。また、真核生物の細胞内あるいは密接に共生する多様な細菌共生体の起源と機能についても研究した。この研究成果は Proc Nat Acad Sci USA（2019 116:15973-15978）に掲載された。

The Inagaki group also collaborated extensively with other researchers, both within and outside the Center. For example, they carried out projects to estimate the interaction between tRNA and proteins involved in translation in *ACS Omega* (2019 4:7308-7316) and developed a software to predict mitochondrion-localized proteins, all in collaborations with other groups of the Center. They also established extensive collaborations with both domestic and interactional partners in various projects.

稲垣教授グループは、センター内外の他の研究者とも幅広く共同研究を行った。例えば、翻訳反応に関与する tRNA とタンパク質の相互作用を推定する研究（ACS Omega 誌に掲載；2019 4:7308-7316））や、ミトコンドリア局在タンパク質を予測するソフトウェアの開発をおこなったが、いずれもセンター内の他グループとの共同研究である。また、

様々な研究において、国内および国外の研究者とのさまざまな共同研究を確立した。

Summary
The molecular evolution group led by Prof. Inagaki is extremely active and the group's research work is highly visible internationally in the field of eukaryotic phylogeny and evolution. Despite its relatively small size, the group managed to be very productive and published quite many research papers in prestigious journals including *PNAS*, etc. The group also established and maintained extensive collaborations with other divisions/groups in the Center as well as with a diverse group of domestic collaborators. The group also has broad international collaborations, including those in Czech Republic, USA, Italy, and France. The group published a total of 47 research papers, 1 conference proceeding and 1 book chapter. The group also received several awards (one domestic and three international). In terms of research funding, the group received many grants and seems to be very well funded. The review committee feels that the group can be further expanded in size and to enhance the effort in developing computational methods to further strengthen the research collaboration with other groups in the Division of Life Sciences and the High-Performance Computational Sciences.

まとめ
稲垣教授を中心とした分子進化グループは非常に活発で、真核生物の系統と進化の分野で国際的にも注目されている。比較的小規模なグループであるにもかかわらず、非常に充実した研究活動を行い、PNAS をはじめとする権威ある学術誌に多数の論文を発表した。また、センターの他部門・グループや国内の多様な研究者との間でも、さまざまな共同研究が行われている。また、チェコ、米国、イタリア、フランスなど幅広い国際共同研究も行っている。当グループは、研究論文 47 編、国際会議論文 1 編、書籍 1 章を発表した。また、いくつかの賞を授与されている（国内 1 件、国際 3 件）。研究資金の面では、多くの助成金を受けており、非常に充実していると思われる。評価委員会では、グループの規模をさらに拡大し、生命科学部門や高性能計算科学部門の他のグループとの研究連携をさらに強化する計算手法開発の取り組みを充実させせることができると考えている。

2.6 Division of Global Environmental Science 地球環境科学部門

This division, headed by Prof. Kusaka, is highly research active and productive. The Review Committee was impressed by the excellent achievements in broader topics in atmospheric science, ranging from urban scale to global scale meteorology and climatology, such as urban climatology, mountain meteorology, atmospheric general circulation, predictability, etc.

日下教授が率いるこの部門は、研究活動が活発で生産性が高い。評価委員会は、都市規模から地球規模の気象・気候学に至るまで、都市気候学、山岳気象学、大気大循環、予測可能性など、大気科学の幅広い分野における優れた成果に感銘を受けた。

The members of the division have established strong international collaborations with NCAR (US), the Oxford University (UK), Indonesia, Sri Lanka. In addition, there are many active researchers who received their Ph.D. from the division and are working in the HPCI community. The Review Committee was impressed with these networks of the researchers, and recommends enhancing these domestic and international collaborations.

この部門のメンバーは、NCAR (米国) 、オックスフォード大学 (英国) 、インドネシア、スリランカと強力な国際協力関係を築いてきた。また、当部門からPh.D.を取得し、HPCIコミュニティで活躍している研究者も多い。評価委員会は、これらの研究者のネットワークに感銘を受け、これらの国内外の協力関係を強化することを推奨する。

The future perspectives include the continuation of ongoing research of computational intensive modeling studies. They include potential contribution to fine-scale weather forecasts for the Tokyo Olympics in 2021. The major works and accomplishments are stated below:

将来の展望は、より強力なモデリング研究を含む。その中には、2021年の東京オリンピックに向けた空間詳細な気象予測への貢献も含まれている。主な成果は以下のとおりである。

i) Urban climatology. Kusaka's group has made significant new progress on the observation and numerical modeling of urban climatology. First, the building-resolving City-LES model is developed with full physics including considering shading and three-dimensional (3D) radiation effects from buildings and trees. In collaboration with relevant groups in CCS, two model codes (an MPI+OpenMP code and a GPU code) are developed, and parallelization with 3D domain decomposition are adopted. This work is cutting edge in both urban climatology and computer science. Second, urban impacts on monthly precipitation amounts in August during a 32-year period are evaluated systematically. Ensemble climate experiments shows urban impact at an increasing rate for each precipitation intensity. These results have the potential influence to the planning of future urbanization, as well as other human developments (e.g., the impact of large-scale solar or wind farms, and the impact of large dams, not only on the water flow but also on the local climate, etc.).

i) 都市気候学 日下教授のグループは、都市気候学の観測と数値モデル化において新たな大きな進捗を得た。はじめに、建物解像都市気象LESモデルを開発した。このモデルは、建物と樹木からの影と三次元 (3 D) 放射効果を考慮することができる。CCSの関連グループと協力して、2つのモデルコード(MPI+OpenMPコードとGPUコード)を開発し、3 次元領域分割法による並列化を適用した。この研究は都市気候学と計算科学の両方で最先端といえる。次に、 32年間の8月の月降水量に対する都市の影響を統計的に評価した。アンサンブル気候実験では、都市が降水に及ぼす影響を弱い降水から強い降水まで、降水強度別に示した。これらの結果は、将来の都市化や他の人間開発(例えば、大規模な太陽光発電所や風力発電所の影響、大規模ダムの影響、水の流れだけでなく地域の気候への影響など)の計画に影響を与えることができるだろう。

ii) Mountain meteorology. Dr. Nishi and Prof. Kusaka focus on the local winds and have made many new achievements in the following two aspects. First, studies of the formation mechanism of Local winds reveal that downslope windstroms are easy to blow due to the bent of the mountains. The convexity of the mountain range has the effect of helping downslope windstorms reach the leeward plain regions. Second, the impacts of foehn winds to extremely high temperatures (EHTs) are thoroughly investigated. The quantitative contributions from foehn winds and urban heat island (UHI) to the EHT events at Niigata are evaluated. These results have high potential impacts to the risk management for strong wind and heat stroke, and to the construction of large infrastructure such as high bridges, etc.

ii) 山岳気象学 西博士と日下教授は、地域の風（局地風）に着目し、次の2つの点で多くの新しい成果を挙げている。第一に、局地風の形成機構の研究は、おろし風の風速が山の曲部により吹きやすくなることを明らかにした。山脈の曲部は、おろし風が風下の平野地域に到達しやすくさせる効果がある。第二に、フェーンの極端高温 (EHT) への影響を丁寧に調べたことである。新潟におけるEHT事象に対するフェーンと都市ヒートアイランド (UHI)の定量的な寄与を個別に評価した。これらの結果は、強風や熱中症のリスク管理や、高架線橋等の大型インフラの建設に大きな影響を与える可能性がある。

iii) Atmospheric general circulation. Prof. Tanaka and Asst. Prof. Matsueda perform simulations with high-resolution global models for atmospheric general circulation studies. The use of the Nonhydrostatic Icosahedral Atmospheric Model (NICAM) on the CCS supercomputer provides a unique outcome of the CCS; O(km) mesh-global simulations have been first conducted by the university computer. The introduction of OpenIFS also is leading prospective research collaborations within CCS and other communities. Their focus on mid- and high-latitudes science, including North Arctic Oscillations (NAO) and blocking, is continuously stimulating the research community. Global high-resolution modeling requires large amounts of computational resources, both of computing time and storage. The Review Committee suggests pursuing more collaboration within CCS and other HPCI community to maximize the activity of global high-resolution modeling studies.

iii) 大気大循環 田中教授と松枝助教は、大気大循環研究のための高分解能全球モデルを用いたシミュレーションを行っている。CCSのスーパーコンピュータ上での非静力学20面体大気モデル (NICAM) の使用は、CCSの独自な結果である。O (km) メッシュでの全球シミュレーションを、筑波大学のスーパーコンピュータで初めて行った。OpenIFSの導入は、CCSやその他のコミュニティ内での共同研究を先導するものでもある。北極圏振動 (NAO) やブロッキングを含む中緯度および高緯度の大気科学への彼らの研究は、研究コミュニティに継続的に刺激を与えている。全球高分解能モデリングは計算時間とメモリの両方の立場で大量の計算資源を必要とする。評価委員会は、世界的な高解像度モデリング研究の活動を最大化するために、CCSおよび他のHPCIコミュニティ内でのさらなる協力を提案する。

iv) Predictability. Atmospheric predictability studies by Asst. Prof. Matsueda with the TIGGE and S2S datasets are highly appreciated by the scientific community. These rich datasets have been used to study the Madden-Julian oscillation, extreme weather including heavy rainfall, the North Atlantic Oscillation (NAO), arctic sea-ice, weather regimes in medium-range forecasts. The archive of these datasets achieves high reputation of the CCS, and are being used by many researchers. They will be grown as representative datasets of the CCS to be open to public, and it is advised that the CCS should consider the best way of maintaining these types of datasets and maximizing their usability.

iv) 予測可能性 TIGGE及びS2Sデータセットを用いた松枝助教による大気予測可能性研究は、本分野の科学コミュニティから高く評価されている。これらの豊富なデータセットは、 Madden-Julian振動、豪雨を含む極端気象、北大西洋振動 (NAO) 、北極海氷、中期予報の気象研究に利用されている。これらのデータセットのアーカイブは、 CCSの高い評価を達成し、多くの研究者によって使用されている。これらはCCSの代表的な

データセットとして公開され、 CCSはこれらのタイプのデータセットを維持し、その有用性を最大化する最良の方法を考慮すべきである。

Summary
Considering the division's excellent scientific achievements in the broad areas so far, the Review Committee had an impression that this division has a great potential to make effective use of more resources both in terms of computational time and to make more impact on the scientific community. Collaborations with computer scientists for better use of the HPC architectures are active and fruitful, but could be improved by having an easier access to technical staff for simpler questions in code development.

まとめ
評価委員会は、当部門のこれまでの幅広い分野での優れた科学的成果を考慮し、この部門が計算時間の面でより多くの資源を有効に活用し、大気科学の研究コミュニティにより大きな影響を与える大きな可能性を持っているという印象を持った。HPC アーキテクチャのより良い利用のためのコンピュータサイエンス研究者との協力は活発で実りあるものである。今後は、コード開発時に気軽に問い合わせができるように、技術スタッフとより簡単にアクセスできるようにすることで、状況はさらに改善することができるだろう。

The CCS at the U. Tsukuba is a highly productive computational science research organization with very strong outcomes. The Division of Global Environmental Sciences is exemplary in this regard. Based on this productivity, the committee would like to see a more aggressive growth agenda for this division. With the potential availability for additional support from the university, what are the strategic areas and topics into which this division should move? We encourage more strategic thinking along these lines.

筑波大学CCSは、非常に優れた成果を上げている生産性の高い計算科学研究機関である。地球環境研究部門はその点で模範的といえよう。この生産性に基づいて、委員会はこの部門のより積極的な成長計画を知っておきたいと考えている。大学から追加的な支援が得られる可能性があるとすれば、この部門が移行すべき戦略的分野とトピックは何か？このような方針に沿ったより戦略的な考えを持つことを推奨する。

Along these same lines of reasoning, the committee would like to see more effective use of the CCS Multidisciplinary Cooperative Research Program (MCRP) to include a larger number of Meteorology and Climate Scientists within the research and user programs and, therefore, exercise greater influence scientifically and programmatically. It is easy to argue that, given the productivity of this group in terms, that the committee is surprised to learn that only ~5% of MCRP compute resources where allocated/used within Global Environmental Sciences. Clearly there is opportunity and reason to grow in this area, and resources should be allocated and plans made in this direction.

委員会は、このような考え方に沿って、CCS学際共同研究プログラム (MCRP) をより効果的に活用し、より多くの気象科学者や気候科学者を研究者プログラムやユーザープログラムに含めることで、科学的かつプログラム的により大きな影響力を与えられるようになるべきと考えている。このグループに対して割り当てられたMCRP計算リソースが全体のわずか5%にすぎないこと、それにも係わらず、このグループの生産性が高い

ことに委員会が驚いている。この分野は今後も成長する機会があり、その理由もあることは明らかであり。このグループに計算資源を配分した上で計画を立てるべきである。

2.7 Division of High Performance Computing Systems 高性能計算システム研究部門

This division acts as the system-side role in the interdisciplinary research collaboration and co-design in CCS. Its research activities cover a wide range of HPC issues including architecture, programming languages, middleware, and numerical algorithms and libraries. The division is also responsible for CCS's HPC systems, HA-PACS, COMA, Oakforest-PACS and Cygnus, specifically, to design, procure and install them as Japan's top-level infrastructure not only for the local use in CCS but also as a key component of HPCI. Another important activity is to pursue international collaborative research projects with US Department of Energy (DoE) laboratories and French and German institutes.

この研究部門は、CCS における学際計算科学研究と co-designing において、計算機システム側の研究を担当している。この部門はアーキテクチャ、プログラミング言語、ミドルウェア、数値計算アルゴリズムとライブラリという、幅広い HPC 研究を展開している。この部門はまた、HA-PACS，COMA，Oakforest-PACS，Cygnus といった CCS におけるスーパーコンピュータ群の運用と、特にその設計、調達、システム導入について、国内最高レベルのシステム構築に貢献しており、CCS 内だけでなく HPCI における重要なコンポーネントとしてそれらを提供する役割も果たしている。また、米国 DoE（エネルギー省）の研究プロジェクトや、フランス及びドイツとの国際共同研究を展開している点も重要である。

Recent architectural research focuses on FPGA computations including GPU/FPGA hybrid computing. The key concept of their research is named Accelerator-in-Switch (AiS). The goal is to make FPGA work complementally with GPU in computations with poor parallelism, poor regularity and/or frequent and latency-sensitive communications. CCS's latest supercomputer Cygnus is designed to investigate the effectiveness of AiS by adding two FPGAs to each of 32 nodes having two CPUs and four GPUs and connecting all of 64 FPGAs with 100Gbps optical link to form an 8x8 2-dimensional torus. Recent research work on AiS focuses mainly on the fundamental communications, namely OpenCL enabled DMA between FPGA and GPU without involving the CPU, and the 2D torus interconnect switch working interactively with OpenCL kernel for applications on FPGA. In addition, a study with a real astrophysics application has been carried out to prove that offloading a part of radiative transfer code from GPU to FPGA is effective when the problem size is small and thus the parallelism is insufficient for GPU computation. In summary, the work on AiS is still preliminary and has not yet proved its excellence due to only one-year experiment with Cygnus, but its high potential based on the high-throughput low-latency communication capability shows promise in the future work with various applications.

最近のアーキテクチャ研究では、FPGA を用いた計算と、GPU と FPGA のハイブリッド利用に関する研究が主なものである。これらの研究の基本概念は AiS（Accelerator-in-Switch : 演算加速と通信ネットワークの融合）と名付けられている。その目的は、FPGA

が GPU の欠点を補完し、相補的な複数デバイスによるハイブリッドシステムを構築し、プログラム内で並列性が不足する箇所や、不規則計算が発生する箇所、通信レイテンシが致命的になる箇所等に対して適切に対応するシステムを開発することである。CCS の最新のスパーコンピュータである Cygnus は、AiS コンセプトの実証実験のために、32 台の計算ノードに各 2 基の FPGA を搭載し、全 64 基の FPGA 間を 100Gbps の光リンクで結合して 8x8 の 2 次元トーラスネットワークを構築している。最新の研究は特にデバイス間通信に着目し、CPU を介さない GPU-FPGA 間の DMA を OpenCL レベルで制御するシステムの開発と、FPGA 間をつなぐ 2 次元トーラスネットワークをやはり OpenCL レベルで利用するシステムの開発、そしてそれらをアプリケーションから利用する技術を中心に行われている。さらに、宇宙物理学の実アプリケーションコードにおいて、GPU だけでは性能が得られない輻射輸送計算に対して FPGA を適用することが、特に GPU の性能を引き出すことが難しい小規模問題において、全体性能を向上させることに成功している。結論として、AiS に関する研究はまだ基礎段階であり、Cygnus の運用開始からは 1 年足らずであることからその実証は十分ではないが、その高い潜在能力と低レイテンシ・高バンド幅の通信能力により、今後様々なアプリケーションの高性能化がなされることが期待される。

The research on middleware for storage and file systems is one of the most prominent efforts in computer science in CCS. Based on the Gfarm file system and Pwrake workflow system, the research product of CCS's own, various projects has been carried out. One direction is to apply them to real big-data analyses such as telescope data processing and homology search for metagenome analysis. Another direction is the enhancement of Gfarm with burst buffers using node-local SSD to achieve 2-3x performance compared to a commercial system, BeeOND. In addition, a scale-out file system for post-peta and exa-scale systems has been proposed with a distributed metadata server and a flash object store. The excellence of these activities is evidenced by more than 40 journal and conference papers and three conference/workshop awards.

ストレージ及びファイルシステムに関するミドルウェア開発は、CCS における計算機科学研究の突出した研究である。Gfarm ファイルシステムと Pwrake ワークフローシステムは CCS 独自のソフトウェア資産であり、様々なプロジェクトに適用されている。研究成果の一つとして、天体望遠鏡のビッグデータ解析やメタゲノムのホモロジー解析への適用がある。また、Gfarm に対して各計算ノードに配備された SSD をローカルストレージとして適用することで、商用システムである BeeOND に比べ 2~3 倍の性能が得られることも示されている。さらに、ポストペタからエクサスケール規模のシステムに対するスケールアウトするファイルシステムでは、分散メタデータサーバとフラッシュオブジェクトデバイスで対応する。これらの研究活動は 40 本以上の雑誌及び国際会議論文として発表され、3 つの学会あるいはワークショップのアワードを受賞している。

As for the research on numerical algorithms and libraries, the division shows the committee steady progress in two topics, namely the FFT and block Krylov subspace method, which have been investigated by division members for many years. The major accomplishment in the former is the implementation of FFTE, a widely used library of CCS's own, on Oakforest-PACS with auto-tuning method. The progress in the latter is the improvement of convergence property, but the linear solver is not yet provided in the form of library.

数値アルゴリズムとライブラリに関する研究については、同研究部門は 2 つの重要な研究成果として、FFT とクリロフ部分空間法についての成果を見せてくれた。これらの研究は同部門の研究者により複数年に渡って蓄積されたものである。FFT についてはFFTE ライブラリとして提供され、CCS の各種アプリケーションに利用され、Oakforest-PACS における自動チューニング手法にも適用されている。クリロフ部分空間法については、精度を保証しつつ反復回数を低減する手法が開発されているが、ライブラリとしての公開には至っていない。

2.8 Division of Computational Informatics 計算情報学研究部門

2.8.1 Database Group データ基盤分野

The Division of Computational Informatics is one of strongest teams on database research in Japan, nation-wide, with 5 faculty members, 2 researchers, 19 PhD/master students, 2 research students, and 6 undergraduate students. This Division serves an important role in the center under the mission of “multidisciplinary computational science” with a focus on big data analytics and AI to support large applications that need high efficient data processing techniques.

計算情報学研究部門は、データベース研究において日本国内で最も強力なチームの一つであり、教員5名、研究員2名、博士・修士大学院生19名、研究生2名、学部生6名からなる。同部門はセンターがミッションとする学際計算科学のもと、ビッグデータやAIにフォーカスし、高度に効率化されたデータ処理技術を必要とする大規模アプリケーションをサポートする上で重要な役割を果たしている。

In the era of big data analytics and AI, the Division of Computational Informatics has focused on information integration framework, data mining and knowledge discovery, as well as the other important perspectives in dealing with various of large amount of data, and provided new techniques to address real issues via collaboration with specialists in different application domains.

ビッグデータ・AI時代において、計算情報学研究部門は、情報統合フレームワーク、データマイニング、知識発見、ならびに多様な大規模データを扱う上で重要な種々の観点に焦点を当て、様々なアプリケーション分野の専門家とも協力しながら、実問題の解決を目指した新たな技術を提供してきた。

Given the nature of computational sciences that deal with simulation, under the information integration framework, the Division of Computational Informatics has conducted research on data stream processing, which also has wide applications in sensors, micro-blogs, etc. The topics covered include smart query execution for event-driven stream processing, incremental continuous queries processing over streams and relations with isolation guarantees, smart distributed query execution over data streams, keyword search over relational streams, architecture for stream OLAP exploiting stream processing engine and OLAP engine, approximate OLAP on sustained data streams, streamingCube, optimization over sequence data, and dynamic spatial-keyword object search. Under the data mining and knowledge discovery, the Division has shown great effort to explore actionable knowledge from massive data. The topics covered include outlier detection, microblog and social media analysis, graph analysis, and non-negative matrix factorization and community detection.

シミュレーションを扱う計算科学の性質を踏まえ、計算情報学研究部門では、情報統合フレームワーク研究の一環として、センサー、マイクロブログ等幅広い応用を有するデータストリーム処理の研究を進めてきた、これに関する研究トピックとしては、イベント駆動型ストリーム処理、隔離性を保証するストリームとリレーションに対する差分連続問合せ処理、データストリームに対するスマート分散問合せ処理、リレーショナルストリームに対するキーワード検索、ストリーム処理エンジンとOLAPエンジンを用いたストリームOLAPアーキテクチャ、永続化されたデータストリームに対する近似OLAP、streamingCube、シークエンスデータの処理最適化、動的空間キーワードオブジェクト検索がある。また、同部門では、データマイニング・知識発見に関して、大規模データから実用的な知識を獲得するため大きなエフォートを充当している。これに関する研究トピックとしては、外れ値検出、マイクロブログやソーシャルメディアの分析、グラフ分析、非負値行列分解、コミュニティ検出がある。

Along the direction of high performance computing, the Division has explored new techniques using advanced hardware such as GPU and FPGA, and has published results related to probabilistic frequent mining on a GPU cluster, GPU-accelerated canopy clustering, GPU-accelerated graph clustering via parallel label propagation, GPU acceleration on set similarity processing, and accelerating regular path queries using FPGA.

同部門では、高性能計算を指向したアプローチとして、GPUやFPGAといった新たな先進的ハードウェアを用いた新たな技術を開拓している。これまで、GPUクラスタを用いた確率的頻出マイニング、GPUによるキャノピークラスタリングの高速化、GPUによる並列ラベル伝搬に基づくグラフクラスタリングの高速化、GPUによる類似集合処理の高速化、FPGAを用いた正規パス問合せの高速化に関する研究成果を論文発表している。

In addition to the main topics on information integration framework, data mining and knowledge discovery, and high performance computing on advanced hardware, there are many other important topics being studied in this Division. One thing that needs to be mentioned is the automated sleep stage scoring. The division has achieved the best sleep stage scoring using the datasets for mice by collaborating with International Institute for Integrative Sleep Medicine. This result has great potential impact on society to fully understand how to deal with sleeping problems for humans.

同部門では、情報統合フレームワーク、データマイニング・知識発見、先進的ハードウェアを用いた高性能計算といった主要トピックに加えて、他の多くの重要なトピックに関する研究も行っている。特筆すべきものの一つとして、自動睡眠ステージングがある。同部門は、国際統合睡眠医科学研究機構と共同で、マウスを対象とした世界最高水準の睡眠ステージ判定を実現した。この研究成果は、ヒトの睡眠に関わる問題の解決を考える上で、大きな社会的インパクトを潜在的に有するものである。

In terms of publication, the division has published a large number of publications including the papers published in major international conferences and renowned journals such as PAKDD, EDBT, ACM CIKM, IEEE ICDE, AAAI, IJCAI, and ACM TSAS. The Division received 14 awards including 8 best paper awards, in the past 6 years. The committee is very impressed by the high quality research being conducted in this Division, for its contribution to the Center and widely to the research communities.

論文発表に関しては、同部門はPAKDD, EDBT, ACM CIKM, IEEE ICDE, AAAI, IJCAI, ACM TSASといった主要な国際会議や著名なジャーナルの論文を含む数多くの論文を発表している。同部門は、過去6年間に8件のベストペーパー賞を含む14件の賞を授与されている。委員会は、同部門で実施されている高い水準の研究と、センターや幅広い研究コミュニティに対する貢献に大いに感銘を受けた。

2.8.2 Computational Media Group
計算メディア分野

Overall the Computational Media Group is performing very well over the review period. The group has published well in academic venues and has an impressive range of stakeholder engagements. These efforts have provided results that have an impact. The research from the group has been successful over the review period, and the future looks very bright for the group.

全体的に、計算メディアグループは、評価期間中に非常に良好なパフォーマンスを発揮している。当該グループは、学術分野でよく論文掲載をしており、研究関係者が関わる分野において印象的な範囲を取り上げている。これらの取り組みにより、周りに影響を与える結果を出している。グループの研究は評価期間中に成功しており、グループの未来は非常に明るく見える。

Examples of good research from the group are the following three projects: 1) Visual Exploration Activity for Read-The-Game Skill Evaluation of Football Players, 2) Bullet-Time Video Effects, and 3) Projector Calibration Method Using a Mobile Camera for Projection Mapping System.

グループからの良い研究事例は、次の 3 つのプロジェクトである: 1)サッカー選手のゲームの読み取りスキル評価のための視覚的探査活動、2)バレットタイムのビデオエフェクト、および 3)プロジェクションマッピングシステムのためのモバイルカメラを使用したプロジェクターキャリブレーション方法。

Visual Exploration Activity for Read-The-Game Skill Evaluation of Football Players. Coaches of the University soccer team approached the group wishing to evaluate a player’s ability to “Read the game”. Visual Exploratory Activity was identified as a main skill for reading the play. The group is actively exploring how to employ this technique with virtual reality and physiological sensors to help train players. VR can be used to optimize training time for coaches and players. Training could be performed outside the normal training field, thus optimizing the use of facilities. The goal is for an easy to use and accessible system that is customizable to different training scenarios. This project is a nice use and fusion of multiple physiological measures. This project has a nice overlap with sports science and can be applied to many other sports. Prof. Koido is a key stakeholder and collaborator; he is one of the coaches of the JFA national team. This project provides a good example of the group’s ability for stakeholder engagement

サッカー選手のゲームの読み取りスキル評価のためのビジュアル探査活動　大学サッカーチームのコーチ達と、「ゲームを読む」選手の能力を評価する本研究グループが連

携している。視覚的な探索的活動は、プレーを読む主要なスキルとして定義される。本グループは、バーチャルリアリティと生理学的センサーの併用によって、この研究をプレイヤー訓練方法にするべく積極的に模索している。VR は、コーチや選手のためのトレーニング時間を最適化するために使用できる。通常のトレーニングフィールド以外でもトレーニングを実施することで、施設の利用を最適化できる。 目標は、さまざまなトレーニングシナリオにカスタマイズ可能な使いやすく、アクセスしやすいシステムの提案である。このプロジェクトは、複数の生理学的尺度の素晴らしい適用と融合である。このプロジェクトはスポーツ科学との重なりが大きく、他の多くのスポーツにも適用できる。小井土先生（※筑波大学蹴球部監督）は、主要なステークホルダーであり、協力者である。彼は JFA のコーチの一人である。このプロジェクトは、ステークホルダーを取り込んで研究することに対するグループの高い能力の一例を示している。

Bullet-Time Video Effects. The Bullet-time video effects is a set of very interesting projects with many research problems to be solved. This is an ideal research direction that has many different angles for investigation. The presentation during the breakout session provided a more complete overview of the projects than the written documentation. The commitee encourages the research to continue in this direction. There are many potential applications of this technique. The initial results provide a good position for stakeholder engagement, as there is an existing useful tool for the end user to explore potential future solutions to their problems. This a good example of the group's work as it is very complete set of research projects to have a comprehensive solution to the problem.

バレットタイム映像エフェクト　バレットタイム映像エフェクトの研究は、解決すべき多くの研究問題を持つ非常に興味深いプロジェクトの集合体である。これは、調査のために、多くの異なる方向性が必要という典型的な研究のあり方の一つである。ブレイクアウト セッション中のプレゼンテーションでは、ドキュメントの説明以上にプロジェクトの概要について詳しく説明があった。評価委員会は、この方向に研究を継続することを奨励する。この手法には多くの潜在的な用途がある。初期的な研究成果は、ステークスホルダーの関与に適した状況を提供できる。それというのも、エンドユーザーには将来の問題に対する潜在的な解決策を検討するための便利なツールが存在するからである。この研究はこの問題に対する包括的なソリューションを持つ研究プロジェクトの完全な集まりであり、本研究グループの成果の良い例であろう。

Projector Calibration Method Using a Mobile Camera for Projection Mapping System. This is a very useful and complete solution to a known problem. The research provided unique solutions, and the team took a novel approach to solve the problem. A particular issue of projector calibration that works in very large areas of projection was solved by their method. A second issue solved is this is a solution that is easy for users to use.

プロジェクションマッピングシステム用モバイルカメラを用いたプロジェクタ校正法
これは、既知の問題に対する非常に有用かつ完全な解決策である。研究はユニークな解決策を提供し、研究者らは問題を解決するために新しいアプローチを採用した。非常に広域の投影領域でのプロジェクタ校正問題は、この方法によって解決された。また、ユーザーが使いやすいソリューションであるように問題が解決されている。

A strength of the group is its strong connections to different parts of the University. The Computer Vision and Image Media Lab is the same as the Media Group. This is important as there is a strong link back into the University. Media Group has a partial overlap with Empowerment Informatics, and this overlap results in good collaborations and helps the research of both research groups. The laboratory space provided to the Media Group is a great asset, and in particular, the Empowerment Informatics large tracked space is very unique in its capabilities. This enables the group to perform novel and innovative research that is not possible for many other international research groups.
本研究グループの強みは、大学の異なる部分との強い接続である。画像情報研究室は、計算メディアグループと同一である。このことは、大学内へ強力なリンクがあるという意味で重要である。計算メディアグループはエンパワーメント情報学と部分的に重複しており、この重複は良好なコラボレーションをもたらし、両方のグループの研究に役立っている。計算メディアグループに提供される実験室スペースは大きな資産であり、特にエンパワーメント情報学の大きなトラッキングスペース（※「ラージスペース」と呼ばれている実験施設のこと）は、その能力において非常にユニークである。これにより、他の多くの国際的な研究グループでは不可能な斬新で革新的な研究を行うことができる。

How does the Computational Media Group measure success?
The Media Group measures success by two categories, academic communication and stakeholder engagement.

計算メディアグループの成功をどのように評価するか?
計算メディアグループについては、アカデミックコミュニケーションとステークホルダーエンゲージメントの 2 つのカテゴリーで成功を評価する。

Academic communication
アカデミックコミュニケーション

The group submits research papers to high-quality computer science conferences and journals, such IEEE International Symposium on Mixed and Augmented Reality, IEEE Virtual Reality, and ACM Journal on Computing and Cultural Heritage (JOCCH). They realize computational media is difficult to publish in these venues, and they work diligently to research problems appropriate for computer science publication venues. They focus on good human computer interfaces in VR and AR. Their approach is adopting and improving on existing results to solve problems for their stakeholders. Their ideal goal is to provide a useful solution to end-users. Many times this requires importing media technology to new application fields. As they stated: "*The technology does not matter, but defeating the problem is most important.*" They are investigating many different fields for applying this technology, such as assistive technology, traffic, culture, education, medical, and sports.

研究論文は、IEEE 複合現実と拡張現実に関する国際シンポジウム(ISMAR)、IEEE バーチャルリアリティ、ACM ジャーナル・オブ・コンピューティングと文化遺産(JOCCH)など、高評価のコンピュータサイエンスカンファレンスやジャーナルで採択されている。これらの分野では計算メディアの研究が認められることが難しいことを認識して

おり、コンピュータサイエンスの学術の場にふさわしい研究となるよう、熱心に取り組んでいる。彼らは、VR と AR における優れたコンピュータインターフェイスに焦点を当てている。彼らのアプローチは、ステークスホルダーの問題を解決するために、既存の結果を採用し、改良するものである。その理想的な目標は、エンドユーザーに有益なソリューションを提供することである。多くの場合、メディアテクノロジを新しいアプリケーション フィールドにインポートする必要がある。彼らが述べたように:「技術が問題ではなく、問題を解決することこそが最も重要である」。 生活支援技術、交通、文化、教育、医療、スポーツなど、この技術を応用するためのさまざまな分野で研究をしている。

They apply a systems-based approach to their research. This entails breaking down their problems to find a good solution. New cutting-edge technology is explored, and novel extensions of the technologies are developed. An example of this is the new combination of EEG and head mounted displays. This is an emerging area of research, and a small number of international researchers are exploring how to use EEG to improve a user's experience in VR and AR. The group is asking the following questions: 1) Which applications do you apply these combined technologies? 2) Is it appropriate? and 3) What kind of VR setting is appropriate?

彼らは研究にシステムベースのアプローチを適用している。良い解決策を見つけるために、問題を分解していく必要がある。新しい最先端技術を探求し、技術の新しい拡張を研究開発している。この例の一つが、EEG とヘッドマウントディスプレイという新しい組み合わせである。これは新たな研究分野であり、VR や AR でのユーザーの経験を向上させるために EEG を使用する方法を模索している研究者はまだ少数である。本研究グループでは次のような質問を取り上げている: 1) どういうアプリケーションにこれらの組み合わせのテクノロジを適用すべきか？2)適用可能か？ 3)どのような VR 応用が適切か?

Stakeholder engagement results impact
ステークホルダーエンゲージメントの結果への影響

The group submits research papers in application domain specific research venues as a means of validation that their work is cutting edge in both computer science and the application domain.

研究論文は、コンピュータサイエンスとアプリケーションドメインの両方で最先端の成果であることを検証する手段として、アプリケーションドメインの研究の場で発表されている。

The group seeks to determine what kind of advantage is available by combining new technologies to solve the end-user's problems, thus maximizing the solution with this combination. This requires an understanding of many emerging technologies.

エンドユーザーの問題を解決するために新しい技術を組み合わせることで、どのような利点があるかを判断し、この組み合わせでソリューションを最適化することを目指している。 このためには、多くの新しい技術を理解する必要がある。

The group has the challenge of determining which application domains would be successful for their research methods. They seek to find the right stakeholder to collaborate with and to find the right domain expert. Once these people are communicating well, they can find the correct problem from them to solve. It must be noted this a difficult challenge for computer science researchers in general. <u>From what the committee can determine, the Computational Media Group has an outstanding record of stakeholder engagement.</u>

この研究グループでは、それぞれの研究手法に対して、どのアプリケーションドメインなら成功を収められるか判断しなくてはならないという課題を抱えている。彼らは、協力関係になるステークスホルダーを適切に見つけ、適切なドメインエキスパートを探すようにしている。これらの人々とうまくコミュニケーションを取ることで、彼らは解決するための正しい問題を見つけ出すことができる。これは、コンピュータサイエンス研究者全般にとって難しい課題である。<u>委員会としては、計算メディアグループは、ステークホルダーエンゲージメントの優れた成果を挙げていると言える。</u>

One method the group employs is to start with a small problem from the stakeholder.　They seek research problems are difficult for all parties. Ideal problems are those that require the expertise of the Media Group and are novel computer science problems. This requires collaboration and joint effort from all parties.

グループが採用する方法の 1 つは、ステークホルダーからの小問題から始めることである。 研究上の課題とは、すべての当事者にとって困難であるような問題である。理想的な課題は、計算メディアグループの専門知識を必要とし、新しいコンピュータサイエンスの問題でもある。これに対するには、すべての当事者からの協力と共同の努力が必要である。

How is the Computational Media Group doing by those measures?
計算メディアグループは、これらの基準にどのように応じているか？

The number and quality of the research papers are good for a group of this size. They are publishing in the correct venues.

研究論文の数と品質は、このサイズのグループに適している。彼らは正しい発表の場を選んで出版している。

Stakeholders appear to be very satisfied with the results. The group has to determine what form of results the stakeholder wish to receive, software, systems or algorithms. This requires compromise from all parties concerning the final results.　This is sometimes in conflict with academic goals, and some effort is required in engineering the final solutions. The group appears to balance these requirements well.

ステークスホルダー達は結果に非常に満足しているように見える。研究者達は、ステークスホルダーが望む結果、ソフトウェア、システム、またはアルゴリズムの形式を決定する必要がある。これを得るには、最終結果に関係するすべての当事者からの合意が必要である。ときには学術的な目標と矛盾する場合があり、最終的なソリューションの生成には努力が必要だ。このグループの研究者らは、これらの要件のバランスをうまく調整しているように見える。

A major metric is the group's current ability to perform technology transfer. The list below provides some examples of their transfer of technology to stakeholders.

主要な指標は、技術移転を実行する能力である。以下のリストは、ステークホルダーに技術移転する例をいくつか示している。

- 2501 Inc has received free point view of video technology from two projects *Multi-Resolution Bullet-Time Effect* and *On-site Visual Feedback Method Using Bullet-Time Video*.
- The project *Proactive Preservation Activity of World Heritage by 3D Reconstruction Technology* is being used by Prof Matsui and potentially used by UNESCO and APSARA National Authority.
- The Nippon Badminton Assoc. provided support for 3D pose analysis of players to improve game analysis, tactics, evidence of training. The technology was installed for the stakeholders.
- The virtual surgery project is in its very early days. There has been a good response up to now from stakeholders.

- 2501 株式会社は、2 つのプロジェクトから自由視点映像技術を受け取っている。*複数解像度のバレットタイム効果*と、*バレットタイム映像を用いたオンサイトビジュアルフィードバック方法*、である。
- *3D 復元技術による世界遺産の積極的保存活動*は、松井教授が活用しており、ユネスコや APSARA 国家機関が利用する可能性がある。
- 日本バドミントン協会は、ゲームの分析、戦術、トレーニングを改善するために、プレイヤーの 3D 姿勢分析をサポートした。この技術はステークスフルダーに導入された。
- 仮想手術プロジェクトは非常に初期の段階にある。これまで、ステークホルダーから良い反応を得ている。

Who are the Computational Media Group's competitors/peers?
計算メディアグループの競合者/仲間は誰か？

The Computational Media Group characterizes the researchers and major laboratories list below as friends, collaborator and sometimes competitors. Japan has a friendly open set of societies in the virtual environments and computer vision research domains. These researchers are happy to exchange ideas and collaborate when the occasion arises. This state of affairs allows for an environment for the Computational Media Group to thrive in its research.

計算メディアグループの特徴として、友人、協力者、時には競合者として以下の研究者と主要な研究所のリストが挙げられる。日本は、仮想環境やコンピュータビジョン研究領域において、友好的でオープンな社会を持っている。これらの研究者は、機会があればアイデアを交換し、喜んで協力している。この状況は、計算メディアグループが研究で繁栄するためのよい環境となっている。

- *Professor Hideo Saito:* Hyper Vision Research Laboratory (HVRL), Keio University, mainly focuses on Computer Vision research.

- *Professor Yoshimitsu Aoki:* Aoki Media Sensing Laboratory, Keio University, conducts research on artificial intelligence technology, computer vision and pattern recognition focusing on image sensing.
- *Professor Hirokazu Kato:* Interactive Media Design Laboratory, NAIST, merges three currently distinct research fields into one: Computer Graphics, Computer Vision, and Human-Computer Interaction.
- *Professor Kiyoshi Kiyokawa:* Cybernetics and Reality Engineering Lab, NAIST, studies virtual reality, augmented reality, and mixed reality focusing on sensing, display and interaction technologies.
- *Associate Professor Daisuke Iwai:* Pattern Measurement Group, Osaka University, investigates virtual reality, augmented reality, human-computer interaction, projection-based augmented reality, and projection mapping.
- *Professor Haruo Takemura:* The Takemura Lab, Osaka University, investigated the following research fields: augmented reality, head mounted displays, user interfaces, robotics, computer vision using machine learning, and e-learning.
- *Professor Iwata Hiroo:* Virtual Reality Lab, University of Tsukuba, investigates intelligent mechanics and mechanical systems that support alternative realities for humans.
- *Professor Masahiko Inami:* Information Somatics, University of Tokyo, designs truly “Human-Computer Integrated” systems enhancing human I/O in a way that we control instruments and systems just like we control our own body.
- *Professor Kiyoharu Aizawa:* Aizawa Laboratory, University of Tokyo, has been working on image and video processing technologies for the next-generation information society.

- 慶應義塾大学斎藤秀雄教授のハイパービジョン研究室(HVRL)は、主にコンピュータビジョン研究に注力している。
- 慶應義塾大学青木義満教授の青木メディアセンシング研究室では、画像センシングに焦点を当てた人工知能技術、コンピュータビジョン、パターン認識に関する研究を行っている。
- NAIST 加藤博一教授のインタラクティブメディアデザイン研究室は、コンピュータグラフィックス、コンピュータビジョン、ヒューマンコンピュータインタラクションの 3 つの研究分野を 1 つに統合している。
- NAIST 清川清教授のサイバネティクス・リアリティエンジニアリング研究室は、センシング、ディスプレイ、インタラクション技術に焦点を当てたバーチャルリアリティ、拡張現実、複合現実を研究している。
- 大阪大学岩井大輔准教授のパターン測定グループは、バーチャルリアリティ、拡張現実、人間とコンピュータの相互作用、投影ベースの拡張現実、プロジェクションマッピングを研究している。
- 大阪大学竹村治雄教授の竹村研究室では、拡張現実感、ヘッドマウントディスプレイ、ユーザーインターフェース、　、 ロボット工学、機械学習を用いたコンピュータビジョン　、e ラーニングなどの研究分野を研究している。
- 筑波大学岩田洋夫教授のバーチャルリアリティ研究室は、人間の代替現実を支える知的力学と機械システムを研究している。
- 東京大学稲見昌彦教授は、人間の I/O を強化する「人間とコンピュータ統合」システム、つまり私たちが自分の体を制御するのと同じように人間の I/O を強化するシステムをデザインしている。
- 東京大学相澤清晴教授の相澤研究室では、次世代情報社会の映像・映像処理技術に取り組んでいる。

Who are the current stakeholders?
現在のステークスホルダーは誰か？

As previously mentioned, the Computational Media Group performs strategic research with real-world impact as a major goal. To perform this form of research, stakeholder engagement is required. They have a history of this form of engagement, and some of the notable stakeholders are as follows: Yahoo Japan Corporation, 2501 Inc., Toyota Motor Corporation, NEC Corporation, Hitachi Ltd., Ministry of Education, Culture, Sports, Science and Technology (MEXT), Nippon Badminton Association, and the Japanese government team for Safeguarding Angkor.

前述のように、計算メディアグループは、現実世界への影響を主要な目標として戦略的研究を行っている。この形態の研究を行うためには、ステークホルダーの関与が必要である。こうした契約の歴史があり、ヤフー株式会社、2501(株)、トヨタ自動車、NEC、日立製作所、文部科学省、日本バドミントン協会、Safeguarding Angkor 世界遺産の日本側関係者などが、この歴史を示す関係者の一部である。

What are the opportunities for international engagement?
国際的な取り組みの機会はどうか？

The Computational Media Group successfully negotiated a set of memorandums of understanding between the Center for Computational Sciences at the University of Tsukuba and the Center for Vision, Speech & Signal Processing at the University of Surrey and Curtin University. These MOUs have strengthened international research relationships for the group.

計算メディアグループにおいては、筑波大学計算科学センターと、サリー大学とカーティン大学ビジョン・音声・信号処理センターとの間で一連の覚書の交渉に成功している。これらの覚書は、グループの国際的な研究関係を強化している。

Looking to the future, the Computational Media Group would like to strengthen its relationship with international sport science researchers. They note this may be difficult across international borders, due to rivalries between nations on the sporting field. The group’s close ties to the University of Tsukuba’s soccer, basketball, baseball teams place them in a good position to work with international sporting researchers, as these teams are considered highly ranked. For example, the national basketball team coach is at the University of Tsukuba.

今後の展望を見据え、国際スポーツ科学研究者との関係を強化したいと彼らは考えている。彼らは、スポーツ分野の国々間のライバル関係のために、国際的な国境を越えての研究は困難であるかもしれないと指摘している。当該グループは、国内で強豪とされる筑波大学のサッカー、バスケットボール、野球部と密接な関係を持ち、国際的なスポーツ研究者と協力する良い位置にいる。例えば、バスケットボールの代表コーチは筑波大学内にいる。

A list of collaborators identified to pursue in 2020 is as follows:
2020 年に協力者としたい者のリストは次の通りである。

- Rio Tinto to investigate 3D computer vision problems with Curtin University,
- Imperial College of London to research 3D virtual surgery,
- Technical Institute of Munich Computer Aided Medical Procedures and Augmented Reality Lab to investigate 3D virtual surgery, and
- Beijing Institute of Technology to investigate AR virtual surgery.

- Rio Tinto は、カーティン大学の 3D コンピュータビジョンの問題を研究している。
- Imperial College of London は、3D 仮想手術を研究している。
- Technical Institute of Munich はコンピュータ支援医療と拡張現実研究室で 3D 仮想手術を研究している。
- Beijing Institute of Technology は AR 仮想手術を研究している。

List of Recommendations
推奨事項の一覧

1. Change the name of the group – The current name Computational Media Group does not reflect the research being performed in the group. One of the external reviewers commented, “I thought the group worked in Journalism.”.
2. Increase the collaboration with other researchers in the CCS – Please continue the good collaboration work and grow these collaborations. The visualization workshop concept presented is a great idea.
3. One potential research area to move into is Immersive Analytics – This research direction fits nicely with the current push in CCS into Big Data and the Media groups AR/VR research directions. The Computational Biomolecular Medicine research is another potential good fit.
4. Make better use of the HPC facilities – Several projects presented have a large computational requirement. Using the CCS capabilities might speed up the research effort.
5. There is a potential overlap with Database Group’s work in streaming data – Real-time video is a form of real-time data streaming. There is potential for the two groups to collaborate on video data processing.

1. グループの名前を変更する – 現在の名前の計算メディア グループには、グループで実行されている研究内容が反映されていない。 外部のレビュアーの一人は、「私はグループがジャーナリズムで働いていると思った」とコメントしていた。
2. CCS の他の研究者との連携を高める – 良いコラボレーション作業を継続し、これらのコラボレーションを成長させること。提示された視覚化ワークショップの概念は素晴らしいアイデアである。
3. 始める可能性のある研究分野の 1 つは没入型分析である – この研究方向は、CCS の現在のビッグデータへのプッシュとメディアグループ AR / VR 研究の方向性にうまく適合する。計算分子医学研究は、もう一つの潜在的な良い組み合わせである。
4. HPC 機能の利用を改善する – いくつかのプロジェクトは、大規模な計算案件を有している。CCS の資源を使用すると、研究の進捗がスピードアップする可能性がある。

5. ストリーミングデータにおけるデータベースグループの仕事と重複する可能性がある- リアルタイムビデオはリアルタイムのデータストリーミングの一形態である。2 つのグループがビデオ データ処理に関して共同作業を行う可能性があろう。

3 Other Center Missions
その他のセンターのミッション

3.1 Overall Evaluation
全体評価

The Review Committee believes that the CCS has created a unique research environment with its strong coupling of applications and computer science code development and emphasis on interdisciplinary computational science research. These collaborations should be continued, and strengthened where possible.

委員会は、CCS が応用科学側研究者と計算機科学側研究者が強く結びつくことにより、独自の研究環境の下でプログラムを開発し、学際計算科学研究を推進していると信ずる。これらの共同研究は継続されるべきであり、より一層強化されるべきである。

The CCS has been a leading proponent of the co-design approach to design computer systems in partnership with applications, which is necessary for advancing computational capabilities. The Cygnus computer system is a great example of the innovative work of CCS in exploring new concepts and ideas for addressing the limitations of current computer architecture approaches, which can only be accomplished in a center where applications and computer science work closely together.

CCS は、co-designing のコンセプトの下、高性能な計算システムを求める応用側研究者との協調作業により、高性能計算機システムの開発を行ってきた。Cygnus システムは、CCS による新しいコンセプトとアイデアにより、現在の計算機アーキテクチャの限界を超えようとする優れた例であり、応用側とシステム側の両研究者集団が強く協調する同センターでこそ実現可能な研究活動である。

The Review Committee welcomes that since 2019 the MCRP allocations on the CCS systems are open for foreign researchers; we recommend the CCS to announce this more broadly to the international computational science community. In order to enhance its international recognition and reputation, we also recommend the CCS to periodically organize international conferences and workshops. In particular, international workshops targeting their (often unique) ‘co-designed’ systems could be valuable to the international community.

委員会は、MCRP（Multidisciplinary Cooperative Research Program：学際共同利用プログラム）が 2019 年から海外研究者にも開かれ、共同利用が可能になったことを歓迎するが、この活動がより広く広報され、国際的な計算科学コミュニティに供されることを推奨する。国際的な認知度を高めるために、CCS が定期的な国際会議及びワークショップを開催することを推奨する。特に、彼ら独自の co-designing されたシステムに注目した国際ワークショップは、国際的研究コミュニティにとって有用であろう。

3.2 Human resource development (researchers) 人材開発（研究者）

The committee finds that the CCS provides a good environment for its staff. The committee does have several concerns, however. Nearly all of the researchers are male, and the committee believes that more needs to be done to address the lack of gender diversity in the research staff. The committee acknowledges that this is a difficult problem, in part because of the demographics in researchers in computing and computational science. However, this is changing, both at leading Universities and in some research organizations. The committee recommends that the CCS look for ways to attract and retain a more diverse group of researchers and staff. For example, it could look to build on its student and visitor programs, and it could use a “climate” survey to evaluate whether there are any unrecognized issues that need to be addressed.

CCS は研究者にとって良好な環境を提供していると思えるが、同時にいくつかの問題が残っていると委員会は考える。ほとんどの研究者が男性であり、研究者のより幅広い性別分散が必要であると考えられる。計算機科学と計算科学分野の人口分布というものがあり、これが難しい問題であることは認識している。しかし、これについては先進的な大学と研究組織において変化が生じつつある。委員会は、CCS が幅広い研究者にとって魅力的であることを訴え、問題を解決する方法を検討することを推奨する。例えば、CCS が学生や訪問者のための良いプログラムを作り、これまで観測できなかったような事項や観点を探し出すような工夫をするとよいと思われる。

One other concern is the age skew in several of the groups, particularly where there are mostly senior researchers near retirement. The committee acknowledges that the CCS is aware of this, and recommends that the CCS develop succession plans for its research leadership, including the efforts to attract and mentor junior researchers to that they can assume leadership of these groups.

もう一つの問題は、いくつかの研究グループで年齢分布が適切でないような例、例えば定年に近いようなシニアな研究者が多いグループが存在することである。委員会は、CCS がこの問題に注意し、センターの魅力をアピールし、若い研究者を指導することで、そういったグループの構成を改善していくように導くことが重要である。

3.3 Student Education 学生教育

The CCS promotes dual degree programs consisting of a doctorate degree in a domain science along with a master's degree in computer science. In addition, courses in ‘Computational Science Literacy' and in ‘High Performance Parallel Computing Techniques for Computational Sciences’ are offered annually; since 2017 both of these courses are offered both in Japanese and in English. The committee commends the CCS for these additions to their curriculum, in particular for offering it in both Japanese and English, and for offering the possibility to obtain a dual degree.

CCS は、科学の各分野の博士課程学生が同時に計算機科学分野の修士課程にも所属し、両分野の学位の取得を目指すデュアルデグリープログラムを進めている。また、「計算

科学リテラシ」と「計算科学のための高性能計算技術」の 2 つのカリキュラムが毎年開設されており、2017 年以降はどちらのクラスも日本語と英語のそれぞれのバージョンが用意されている。委員会は、これらのカリキュラムに加え、デュアルデグリープログラムの全てのコースが日本語と英語に対応することを推奨する。

CCS Report: PART I

Overview of
Center for Computational Sciences

Summary of Activities

2014 – 2019

February 2020

Center for Computational Sciences
University of Tsukuba

Table of Contents

1 Introduction

This report summarizes the main events and activities of the Center for Computational Sciences (CCS), University of Tsukuba, from April 2014 to January 2020. The report has been prepared for the external review of CCS, which is scheduled from February 19th to 21st in 2020.

The purpose of the review is to receive an outside examination of the research activities and their outcomes at the CCS in view of the founding objectives, and to incorporate the recommendations from the review into future developments of the CCS.

Since the details of the research results are prepared as a separate report, this PART I of the reports focuses on an overview, which includes a brief overview and the mission of the CCS (Section 2), organization and administration (Section 3), a chronicle (Section 4), and a brief summary of the research activities and collaborations of the Center (Section 5). More details of the research activities and results in each research division and group are described in the CCS Report: PART II. The future plan and vision are described in CCS Report: PART III.

2 Mission and Overview of the Center for Computational Sciences

Computational science, which is defined as the exploration of science by means of computers, is an indispensable research methodology in the basic and applied sciences, and contributes significantly to the progress of a wide variety of scientific research fields. The mission of the Center for Computational Sciences (CCS) is the promotion of "Multidisciplinary Computational Science" through enhanced cooperation between, and the fusion of, computational and computer sciences. To that end, the CCS works toward the development of high-performance computing systems and networks, conducts sophisticated simulations in a variety of scientific research fields, and endeavors to expand the frontiers of Big Data analysis and innovative information technology. Our scheme of designing and implementation of supercomputers dedicated to various coverage of our application research fields has been done through tightly coupled discussion between domain scientists and computer scientists, which is known as "codesigning" today. Our center has been continuing this codesign manner of collaboration between these fields before this word is widely used as in today.

The scientific research areas of the CCS encompass particle physics, astrophysics, nuclear physics, quantum condensed matter physics, life science, and environmental science. To realize the high-speed, large-scale simulations required in these research areas, the CCS works continuously to develop new state-of-the-art computing systems and networks, while also striving to advance cutting-edge knowledge in computational intelligence with database and media technology. Since FY2013, the CCS was authorized as one of the two prime research centers in University of Tsukuba by "Organization for the Support and Development Strategic Initiatives", and from FY2017, the CCS was ranked as R1 Center of which goal is to establish the world top class research on every research field in computational sciences and high performance computing.

The CCS has a history of 28 years, which is shown in the chronology of CCS (Section 4). It was originally formed as the Center for Computational Physics (CCP) in 1992, then it was reorganized and relaunched under its current name of Center for Computational Sciences (CCS) in April 2004. Currently, the CCS is known as one of the world's leading research institutes engaged in the pursuit of the abovementioned fields, and is also a notable joint-use facility for outside researchers. In all of our target areas, the CCS plays a significant role in the development of the Multidisciplinary Computational Science which we define as an ideal collaboration among all sorts of computational science and engineering and high performance computing technology. It implies not just collaborations between science and technology, but also interdisciplinary collaborations between different fields of scientific researches.

Since 2010, the CCS has been approved as a “national core-center” under the Advanced Interdisciplinary Computational Science Collaboration Initiative (AISCI) launched by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan, and has provided the use of its computational facilities to researchers nationwide as part of the Multidisciplinary Joint-use Program. Furthermore, as part of efforts aimed at supporting collaboration in multidisciplinary computational science, the CCS welcomes applications for scientific meetings, hosts talented researchers from overseas, and strives to locate and retain short-term auxiliary supporters. All these efforts combine to create a strong bridge between domestic and international collaborations, while promoting the interchange of researchers and students. Besides of our original supercomputer resource sharing program named Multidisciplinary Collaborative Research Program, a large portion of our supercomputer resources are dedicated to the general supercomputer sharing program under the name of High Performance Computing Infrastructure (HPCI) by MEXT.

Also in 2010, the CCS was recognized as an affiliated institute of the HPCI Strategic Program Field 5 “Origin of Matter and the Universe”, which aims to further advance the computational sciences using “K” Computer technology. After this strategic program ended with the completion of “K” Computer development, the CCS was selected again for the Important Application Development Program Field 9 “Fundamental Science” toward the application development for "Post-K" Computer which was finally named "Fugaku".

So far, the CCS has developed computers best suited for scientific exploration based on cooperation between computational and computer scientists, as known as "codesigning". Our "Multidisciplinary Computational Science” is one of the real implementations of codesigning of supercomputers and their applications. Its history started in 1996 with our development of the massively parallel supercomputer named the Computational Physics by Parallel Array Computer System (CP-PACS [PACS-VI]), which was ranked as the No. 1 system on the Top 500 List of November 1996. Our codesigning spirit guided us to the following supercomputers such as Parallel Array Computer System for Computational Sciences (PACS-CS [PACS-VII], 2006), a special purpose parallel system for astrophysics named FIRST (2007), the first GPU accelerated supercomputer named Highly Accelerated Parallel Computer for Computational Sciences (HA-

PACS [PACS-VIII], 2011), and the many-core architecture supercomputer named Cluster Of Many-core Architecture processor (COMA [PACS-IX], 2013). While we developed these original supercomputers under the name of traditional "PACS" series, we also collaborated with other two national universities, the University of Tokyo and Kyoto University, to align for general purpose large scale supercomputer specification and operation under the name of "T2K (Tsukuba-Tokyo-Kyoto) Alliance". Its purpose was to introduce three supercomputers in these universities where the basic specification such as CPU type and performance, interconnection performance, memory performance and so on, for widely spread application development and running. T2K Alliance was operated under the concept of "Open Supercomputer" which renewed the traditional supercomputer procurement style in Japanese national universities which had been depending on the vendor-oriented supercomputers.

During our experience on how to apply the accelerated supercomputing to various applications, we proposed a conceptual design of high-performance and low-power accelerated computing with ultra-wide SIMD architecture toward Exascale Computing which was named EXtremely Accelerated Computer (EXAC) in the feasibility study under MEXT for Exascale Computing. This feasibility study purposed the conceptual design of Post-K Computer, however our proposal was not accepted by MEXT unfortunately. Although we could not play the central role of Post-K Computer development, our experience on codesigning contributed to the design and implementation of Fugaku supercomputer as a member of research group.

Collaborations and alliances in computational science research are important factors for promoting and accelerating interdisciplinary computational science. To that end, we have strengthened international collaborations through alliances with The University of Edinburgh in the UK and Lawrence Berkeley National Laboratory in the US. We are also promoting the International Lattice Data Grid (ILDG), which is an international project aimed at the development of data grids for sharing lattice quantum chromodynamic (QCD) configurations worldwide. An XML-based markup language, QCDml, which describes metadata for QCD configurations and ensembles (sets of configurations with common physics parameters), has been developed. The construction of regional ILDG grids has been finalized in the US, UK, Germany, Australia, and Japan [where it is known as the Japan Lattice Data Grid (JLDG)].

After T2K Alliance successfully completed with the end of the life of three machines in three universities, in 2013, we joined with the University of Tokyo again in establishing the Joint Center for Advanced HPC (JCAHPC) as the first interuniversity joint-use center in Japan, which is targeting at the construction of an unprecedentedly large-scale computational facility. In JCAHPC organization, we decided to merge our supercomputer procurement budget of two universities to realize the fastest supercomputer in Japan which exceeds the performance of K

Computer, the ex-fastest one in Japan. Finally, we successfully introduced the Oakforest-PACS (OFP) supercomputer as the first machine of JCAHPC in 2016, with 25PFLOPS of peak performance which was 2.5x faster than K Computer.

Furthermore, since our university is located in Tsukuba Science City, which is home to many government research organizations, we already have firm connections to a number of major research institutions located there. These include the High Energy Accelerator Research Organization (KEK), the Advanced Institute for Science and Technology (AIST), the National Institute for Materials Science (NIMS), the Meteorological Research Institute (MRI), and the National Institute for Environmental Studies (NIES).

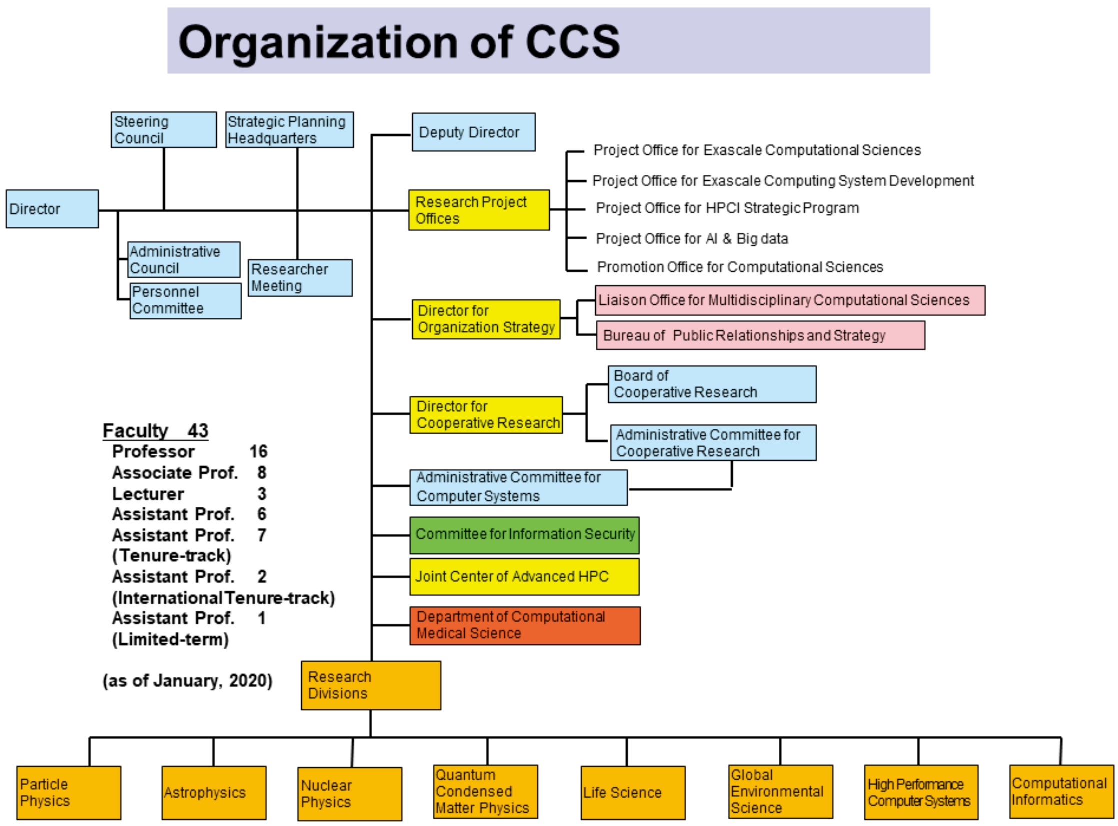
Picture of main building of Center for Computational Sciences

Picture of extended building of Center for Computational Sciences

3 Organization and Administration

3.1 Organization & Operation

The research activities of the CCS are organized under the leadership of the Director with the support provided by the Administrative Office. The organization and the roles of meetings in the CCS are as follows.



✧ Director

The Director of the Center has to hold the rank of professor of University of Tsukuba. The Director is appointed by the President of University of Tsukuba; in practice, a candidate is selected by a ballot of the Center faculty. The appointment is for two years and can be repeated up to six years. The past directors are Prof. Yoichi Iwasaki (particle physicist) from April 1992 to March 1998, Prof. Akira Ukawa (particle physicist) from April 1998 to March 2007, Prof. Mitsuhisa Sato (computer scientist) from April 2007 to March 2013, and Prof. Masayuki Umemura (astrophysics) from April 2014 to March 2019. The current director since April 2019 is Prof. Taisuke Boku (computer science).

✧ Steering Council

The council is held twice a year, and the chair is selected from outside of U. Tsukuba. The council reviews the research activities in each field and the collaborations based on the multidisciplinary joint-use program, and discusses the direction of research of the Center and matters related to joint-use of the Center facility.

✧ Administrative Council

The Director of the Center chairs the council, which holds a meeting every month. The committee discusses significant issues for operating the Center, which include matters related to the organization of the Center, selection of faculty members, budget planning, and confirmation of expenditures.

✧ Strategic Planning Headquarters

The headquarters is planning the requests for budgetary appropriations and faculty members for the enhancement of research activities as well as international collaborations.

✧ Researchers Meeting

This meeting consists of the entire Center faculty, Post-Doc members and the Associated Research Fellows. This meeting is chaired by the Director of the Center and is held every month. At the meeting, all aspects of research are discussed, such as the status of ongoing projects, research activities of all divisions, procurement of equipment and operation of the Center computer system.

✧ Research Project Offices

These offices propel the missions regarding the challenge to novel computer technology, the multidisciplinary collaborations, and the nationwide/worldwide promotion of computational science. The following offices are set up (see Subsections in Section 5.7):

- ✦Project Office for Exascale Computational Sciences
- ✦Project Office for Exascale Computing System Development
- ✦Project Office for HPCI Strategic Program
- ✦Liaison Office for Multidisciplinary Computational Sciences
- ✦Promotion Office for Computational Sciences
- ✦Project Office for AI & Big Data

✧ Department of Computational Medical Science

Since 2019, the CCS launched a new research complex named Department of Computational Medical Science as a collaborative research framework over science, medical and engineering researches. "Department" is a new framework in the CCS which provides a crossing-field research collaboration among various research divisions such as life science, astrophysics, database, media informatics, and also with other section of U. Tsukuba such as Cybernics Center, International Institute for Integrative Sleep Medicine (IIIS) and Department of Medicine.

(see Section 5.7.5 for the details)

✧ Administrative Committee for Cooperative Research

The CCS is calling for applications once a year for the joint-use program of computer facilities. Since 2007, these activities have been reinforced by enhanced links with computer sciences through the promotion of the Multidisciplinary Cooperative Research Program (MCRP). Since 2010, the Center has been recognized as a national core-center under the Advanced Interdisciplinary Computational Science Collaboration Initiative (AISCI) by the MEXT. The administrative committee manages this joint-use program.

(see Section 5.5 for the details)

✧ Bureau of Public Relations

In 2010, the bureau was initiated aimed at improving relations with society in order to advance the mission of the CCS and to expand the public outreach. The bureau organizes the opening to the public every year, and also guides visitors at various kinds of events.

(see Section 5.7.8 for the details)

✧ Research Divisions

The specific researches in each field are promoted in the following divisions:

- ✦Particle Physics
- ✦Astrophysics
- ✦Nuclear Physics
- ✦Quantum Condensed Matter Physics
- ✦Life Sciences
- ✦Global Environmental Science
- ✦High Performance Computer Systems
- ✦Computational Informatics

(see Part II for the details)

3.2 Faculty of the Center

The faculty members belong to the Center and also work at one of eight graduate schools at the University of Tsukuba.

The faculty members as of January 2020 are listed in Appendix A.

3.3 Faculty Selection

The Center appoints new faculty members when openings become available among the Center faculty positions. The selection procedure is as follows.

- Choice of field

When an opening of a position becomes available, the field of the position is chosen by the Personnel Committee based on consideration of the strategic purposes of the Center and the balance among research fields.

- Selection of candidate

Once the field is chosen, the actual selection process is handled by the Faculty Selection Committee under the Personnel Committee. The opening is publicly announced to invite applications. Candidates are initially screened by the Faculty Selection Committee. This screening includes reading the candidates' main papers and interviews. When the screening at the committee converges toward a candidate, the conclusion is reported to the Personnel Committee. If the Personnel Committee approves the candidate, the result is reported both to the Administrative Council and the University Personnel Committee for official approval.

4 Chronicle of CCS

The chronicle of the Center for Computational Sciences goes back to 1992, when the Center for Computational Physics (CCP) was founded at University of Tsukuba. The purpose of the CCP was (i) to carry out research and development of parallel computers suitable for large-scale computational physics calculations, and (ii) to carry out research with the developed system in the area of particle physics, astrophysics, and condensed matter physics. In particular, the CCP was to serve as the base for the project entitled "Research of Field Physics with Dedicated Parallel Computers" (FY1992-FY1996) funded by the Ministry of Education of the Japanese Government. This project developed a massively parallel system CP-PACS (Computational Physics with Parallel Array Computer System). This system achieved 368.2 Gflops for the Linpack Benchmark in September 1996, and was ranked as the No. 1 system in the November 1996 Top 500 List. CCP had a faculty of 10 researchers in four divisions: Computational Particle Physics, Computational Astrophysics, Computational Condensed Matter Physics and Parallel Computer Engineering. The simultaneous existence of physics and computer science faculties within the CCP, and actual close collaborations between them for the development of parallel computer systems and their usage, marked the unique feature of the Center. In fact, this interdisciplinary approach goes back to the early 1980s, when research and development of parallel computer systems started at University of Tsukuba under Professor Tsutomu Hoshino. The CP-PACS is the 6th generation of PAX/PACS series. In the late 1990s, large-scale calculations using CP-PACS produced a number of well-known results. The major scientific achievements are as follows:

1. Calculation of the quenched light hadron spectrum in lattice quantum chromodynamics (QCD). (S. Aoki et al., Physical Review Letters 84 (2000) 238)
2. First systematic lattice QCD calculation including light dynamical up and down quarks, showing that up and down quark masses are much lighter than previously thought. (S. Aoki et al., Physical Review Letters 85 (2000) 4674)
3. First astrophysical radiation hydrodynamical calculation of the reionization of the Universe including the interaction of radiation and matter. (T. Nakamoto et al., Monthly Notice of the Royal Astronomical Society 321 (2001) 593)

4. First many-body quantum mechanical calculation of the phases of solid hydrogen. (H. Kitamura et al., Nature 404 (2000) 259)

In April 2004, the Japanese national university system, of which University of Tsukuba is a member, underwent a major transition. While previously the national universities were part of the Japanese government and were strictly controlled by the Ministry of Education, Science, Culture and Sports, their legal status was changed to that of independent institutes. While the budget still came from the government, each university was granted much wider freedom of action on its own. The reason behind this change was pressure toward the reformation of the Japanese government, including not only a reduction of employees and government spending, but also reformation of the university system to be more effective in the era of globalization and worldwide competition. Preparations for the transition started in FY2002 at all national universities across Japan. The Center for Computational Physics considered the transition as a welcome opportunity to reexamine its future plan. While the Center for Computational Physics, with its small faculty of a dozen members, had functioned well in pursuing research projects within a limited area of fundamental physics, it was strongly felt that the interdisciplinary approach toward computational physics pursued at the Center could be extended to wider areas of science, and that the Center had a potential to significantly expand its activity by doing so. Discussions with the Executive Office of the University on a possible reorganization and expansion started in the early summer of 2002. The Executive Office basically welcomed the Center’s proposal, and provided strong support during negotiations with the Ministry of Education, Science, Culture and Sports to secure governmental approval from the winter of 2002 to the spring of 2003.

The Center for Computational Physics was formally reorganized as the Center for Computational Sciences on 1 April 2004. The faculty expanded threefold from 11 to 31 academic members, and the following reorganization and expansion of divisions were accomplished:

- Division of Particle Physics and Division of Astrophysics were combined into a single division with an increased faculty of 7 members.
- Division of Condensed Matter Physics and Division of Biophysics were combined and significantly expanded to 10 faculty members in the Division of Materials and Life Sciences.
- A new Division of Global Environment and Biological Sciences was introduced with 3 faculty members.
- Division of Parallel Computer Science was expanded from 3 to 5 faculty members, and was renamed Division of High Performance Computing Systems.
- A new Division of Computational Informatics with 6 faculty members was set up to carry out research on computational intelligence and media.

Of the 20 members added to the original 11 for the Center for Computational Sciences, 14 were faculty members who were actively working in various areas of computational science at graduate schools of the university, while the remaining 6 were approved by the university and filled by new recruitments in 2004-2005.

Gordon Bell Prize 2011 for Peak Performance (University of Tsukuba, University of Tokyo, RIKEN) in an atomic state simulation at actual semiconductor device scale. Gordon Bell Prize 2012 (University of Tsukuba, RIKEN, Tokyo Institute of Technology) for scalability and sustained performance in a world's largest scale of a dark matter simulation.

The CCS has been continuing supercomputer development of PAX/PACS series systems. In November 2013, HA-PACS/TCA was added to HA-PACS system and the entire system performance reached 1.166 Pflops. In 2014, the second Pflops-class supercomputer COMA (Cluster of Many-core Architecture) started its operation. HA-PACS and HA-PACS/TCA was a PC cluster with GPU accelerators, and COMA was an accelerated supercomputer with many-core architecture. In April 2019, Cygnus which is the next generations accelerated supercomputer with GPU and FPGA was installed and started its operation based on our experiences on HA-PACS and HA-PACS/TCA.

In 2013, we established the Joint Center for Advanced HPC (JCAHPC) with the University of Tokyo, which is aiming at the construction of an unprecedentedly large-scale computational facility. In December 2016, Oakforest-PACS which is operated by JCAHPC started its operation.

The CCS was authorized as one of the two prime research centers in University of Tsukuba by “Organization for the Support and Development Strategic Initiatives” in 2013. Also, the CCS was reorganized towards more strategic goals with setting up Research Project Offices. In 2015, the Division of Astrophysics and Nuclear Physics divided into two divisions respectively. In the following year, the CCS was positioned as an independent organization obtaining the authority to manage personnel affairs and budgets.

Chronology of CCS

1992	April	CP-PACS Project begins (5-year project). Center for Computational Physics (CCP) founded (10-year term).
1993	August	Computer building completed
1995	March	First research building completed
1996	September	CP-PACS (2048 PU) completed and installed
	November	Ranked as No. 1 on the Top 500 World Supercomputer List
1997	April	Research for the Future Program "Development of Next-Generation Massively Parallel Computers" begins (5-year term)
2002	April	Second 10-year term of the Center for Computational Physics begins
2004	April	CCP is reorganized, expanded and relaunched as the Center for Computational Sciences (CCS)
2005	April	Development of Massively Parallel Cluster PACS-CS in the project begins (3-year term)
2007	March	Second research building completed
	April	Cosmo-Simulator FIRST completed and installed
2008	June	Operation of T2K-Tsukuba begins.
2010	April	Approved under the Advanced Interdisciplinary Computational Science Collaboration Initiative (AISCI) CCS is reorganized from five to seven divisions
2011	November	Gordon Bell Prize 2011 for Peak Performance (University of Tsukuba, the University of Tokyo, RIKEN)
2012	February	HA-PACS starts operation
	November	Gordon Bell Prize 2012 (University of Tsukuba, RIKEN, Tokyo Institute of Technology) for Scalability and Sustained Performance
2013	March	Joint Center for Advanced HPC established in alliance with the University of Tokyo
	April	Reorganized towards strategic goals
	August	Authorized as one of the two prime research centers in U. Tsukuba
	November	HA-PACS/TCA is added to HA-PACS system and ranked No.3 in the Green 500 list
2014	April	COMA (PACS-IX) is installed and starts operations
2015	April	CCS is reorganized from seven to eight divisions
2016	December	Oakforest-PACS is installed and starts its operations in JCAHPC
2019	April	Cygnus is installed and starts operations

Supercomputers in CCS

QCDPAX（1990-1999/3）

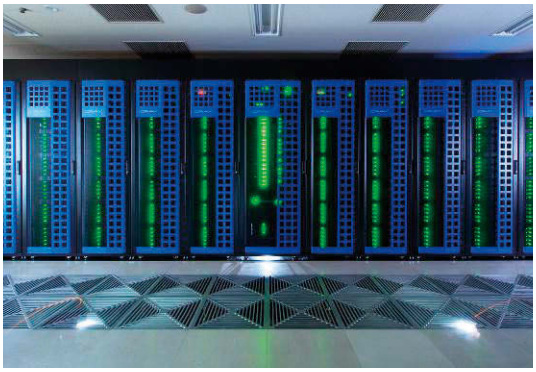
CP-PACS（1996/3-2005/9）

PACS-CS（2006/7-2011/9）

FIRST（2005/3-2013/3）

T2K-Tsukuba（2008/6-2014/2）

HA-PACS（2012/2-2018/10）



COMA（2014/4-2019/3）

Oakforest-PACS（2016/12-）

Cygnus (2019/4-)

5 Overview of Research Activities from 2014 to 2019

5.1 HA-PACS Project

Motivation and Objective

After the end of PACS-CS Project, the accelerated computing represented by GPGPU technology has been focused as one of the solutions to high performance/power ratio in the future HPC systems. GPU became the most inexpensive device to provide very high peak performance and memory bandwidth with relatively low power consumption especially after NVIDIA started to provide CUDA environment for easy and portable programming method. However, GPU solution implies a number of problems such as low bandwidth on communication with CPU and external communication devices due to the bottleneck by PCIe (PCI Express) channel, limited memory capacity, long latency of communication, complicated programming, etc.

As a solution to communication performance issues and programmability, we launched a new project named HA-PACS (Highly Accelerated Parallel Advanced system for Computational Sciences) as MEXT supported project from FY2011 to FY2013. We focused on the commodity communication channel of PCIe to connect all the peripherals including GPU, Ethernet, HCA or HDD. PCIe is originally a communication channel under master control by host CPU (RootComplex) where all the peripheral devices work as slaves (Endpoints). The communication among GPUs on different computation nodes must be performed through CPU memory and its support. For example, MPI function is called for external communication among nodes by host CPU with before/after communication between CPU and GPU within the node. If we have an active and intelligent PCIe switch instead of passive switch, it is theoretically possible to enable the active communication between GPUs without overhead of data copy, and low latency and high bandwidth on inter-GPU communication are realized. For the next generation of large scale GPU clusters, such a sophisticated interconnection network is required, especially for strong scaling parallelization.

This concept is named TCA (Tightly Coupled Accelerators) as the basic idea of HA-PACS system. Fig. 1 shows the difference between ordinary inter-node communication among GPUs and communication based on TCA.

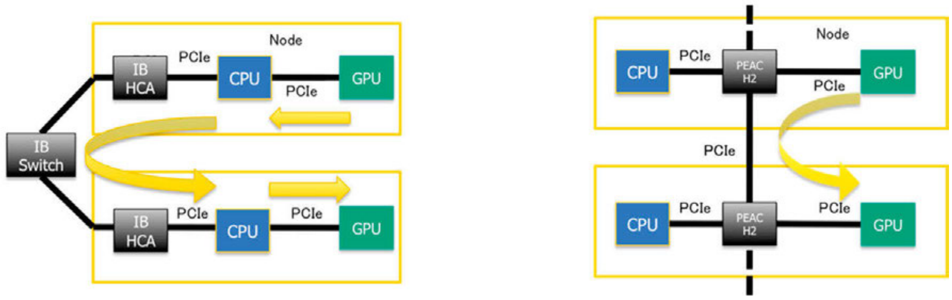


Fig. 1 Traditional inter-node communication between GPUs on GPU clusters (left) and the method in TCA (right)

The objective of HA-PACS project is (1) establishing the elementary technology to enable accelerator device to device (ex. GPU) direct communication on intelligent PCIe switch, and (2) developing the basic algorithm and code for several specially focused application fields under TCA concept. Especially, the second objective is important as the basic algorithmic enhancement or renewal of traditional simulation codes to be ready for next generation supercomputers with advanced accelerated computing. As the Feasibility Study on next generation supercomputer, CCS and collaborative team are proposing very wide SIMD accelerator architecture for the computing element (see the section of Feasibility Study in this report), and we need a drastic model/algorithm change for next generation. We consider that the algorithms modified based on TCA concept take important roles there.

Not only for development of hardware/software on TCA concept, we also introduce a large scale GPU cluster system for basic development, evaluation and produc-running of various codes developed in CCS. Since TCA architecture research is undergoing, we introduce two systems in HA-PACS Project. The first one is named HA-APCS Base Cluster and the latter is named HA-PACS/TCA.

System Overview

Since the development of the communication devices based on TCA concept takes approximately one year, we first installed HA-APCS Base Cluster (“Base Cluster” hereafter) as a commodity GPU cluster with the latest technologies. It was delivered and started the operation on February 2012. This delivery timing allowed us to introduce the advanced CPU of Intel Xeon E5-2670 (SandyBridge) as the host CPU and NVIDIA M2090 (the last version of Fermi) as GPUs on each node. We employed two sockets of CPUs and four GPUs on each node because SandyBridge architecture provides PCIe gen.3 x40 lanes at maximum per CPU and two sockets of them theoretically provide x80 lanes in total. That is enough to connect four GPUs each of them requires PCIe gen.2 x16 lanes. We also employed dual rail InfiniBand QDR HCA supported by PCIe gen.3 x8 lanes to provide 56Gbps of maximum performance for interconnection network.

Fig. 2 shows the overview of Base Cluster and TCA part, and Fig. 3 shows the picture of computation node and its block diagram. Table 1 shows the basic specification of Base Cluster.

Fig. 2 Overview of HA-PACS Base Cluster and TCA part (five racks of front side are for TCA part and others are for Base Cluster)

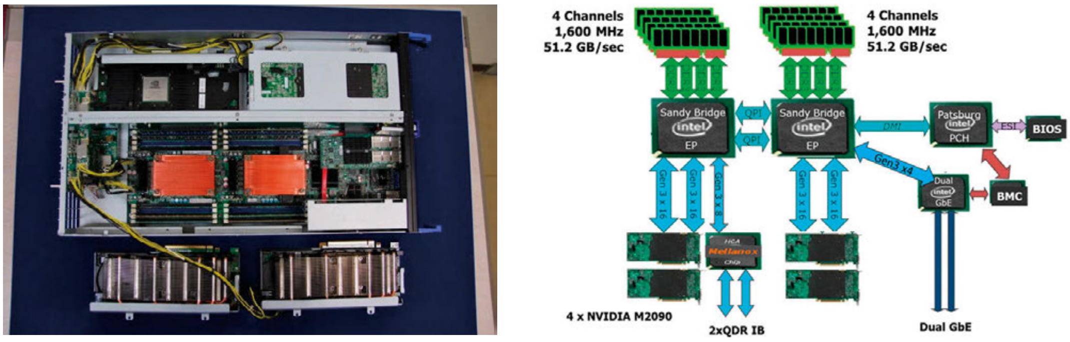


Fig. 3 Computation node and its block diagram of HA-PACS Base Cluster

HA-PACS/TCA was introduced later on October 2013 with a dedicated PCIe extension card for TCA architecture and connected to the central InfiniBand switch with Base Cluster. The basic node configuration of TCA part is same as that of Base Cluster, except CPU is Intel Xeon E5-2670v2 (Ivy Bridge) and GPU is NVIDIA K20X (Kepler) for greater performance enhancement. Main memory bus speed is also upgraded to 1866MHz. In total, the peak performance of computation node in TCA part is 5.69 TFLOPS (348 GFLOPS by CPU and 5320 GFLOPS by

GPU), and the total peak performance of TCA part with 64 nodes reaches 364 TFLOPS. We can run Base Cluster and TCA part as a single system although these CPUs and GPUs are different, and the entire system performance is 1.166 PFLOPS as peak.

Each computation node of TCA part consists of a PCIe card named "TCA Board" to contain an FPGA chip and its peripherals including three ports of PCIe extended connection link to connect with other nodes. We employed FPGA technology to realize TCA architecture because we need to enhance its function and performance.

Table 1 Basic specification of HA-PACS Base Cluster

Computation node (Base Cluster)	CPU	Intel Xeon E5-2670, 2.6 GHz x2 socket
	# of cores	16 (8 cores / CPU)
	GPU	NVIDIA M2090 (Fermi) x4
	Main memory	128GB (DDR3 1600MHz x 16)
	GPU memory	24GB (6GB / GPU)
	Peak performance	332.8 GFLOPS (CPU) + 2660 GFLOPS (GPU)
Computation node (TCA)	CPU	Intel Xeon E5-2670v2, 2.8 GHz x2 socket
	# of cores	20 (10 cores / CPU)
	GPU	NVIDIA K20X (Kepler) x4
	Main memory	128GB (DDR3 1866MHz x 16)
	GPU memory	24GB (6GB / GPU)
	Peak performance	448 GFLOPS (CPU) + 5240 GFLOPS (GPU)
Computaion node (common)	Network HCA	InfiniBand QDR x 2 rail (Mellanox)
	Peak network b/w	7 GB/s
Number of nodes		268
Interconnection configuration		Fat-Tree with full bisection b/w
Peak performance		802 TFLOPS
Network bisection b/w		1.88 TB/s
Shared file system		RAID6 with Lustre (DDN)
File system capacity		500TB (user)

This FPGA chip for TCA architecture is named "PEACH2 (PCI Express Adaptive Communication Hub ver.2)". The name of PEACH is inherited from our previous research in JST/CREST to utilize PCIe link as low power and high performance reliable link for embedded systems (see HPCS Division's section in this report). Fig. 4 shows the picture of PEACH2 card.

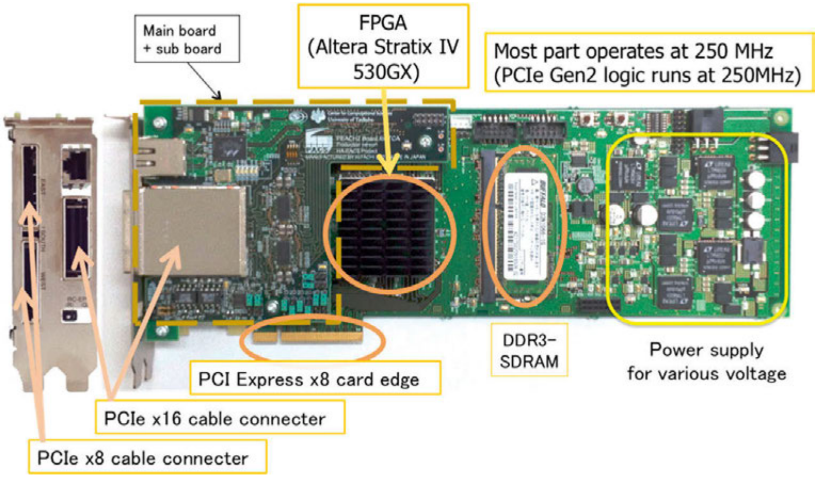


Fig. 4 PEACH2 Board for TCA architecture

The operating system of HA-PACS is Red Hat Enterprise Linux and we employ MVAPICH2, NVIDIA CUDA, CUBLAS, PGI compiler (C/C++/Fortran for CUDA), Intel compiler for GPU, OpenMP and MPI programming environment.

For the programming on TCA communication, we provide a special API to allocate and map the transfer target memory, set-up the communication such as RDMA transaction, and invoke the communication. To perform the memory to memory copy between GPUs on different nodes, we need the information on CUDA bios and memory map on system side. For this purpose, we made an NDA with NVIDIA to share the information required for R&D of TCA and PEACH2.

We measured HPL performance on Base Cluster and TCA part individually since the installation time differs and it is difficult to make a good balance on load between two types of GPUs where the new one provides approximately doubled performance of the older although entire system including two parts can be operated as a big cluster. We recorded HPL score individually to TOP500 site, and HA-PACS Base Cluster was ranked at #41 on TOP500 list on June 2012 with 421.6 TFLOPS of HPL score. TCA part was ranked at #134 on TOP500 list on November 2013 with 277.1 TFLOPS. The score by Basic Cluster is reasonable as a commodity GPU cluster but it is shown that PCIe to support four GPUs per node is not the bottleneck in the performance thanks to rich configuration of Intel Xeon Sandy Bridge or Ivy Bridge. The HPL efficiency is especially high on TCA part corresponding to 76% of the peak performance. Thanks to its low power consumption, HA-PACS/TCA was ranked at #3 in Green500 list on November 2013. Since the PEACH2 board is under tuning, we did not employ it for parallel processing on HPL measurement, and we used MVAPICH2 with dual rail of InfiniBand QDR.

Operation

Base Cluster started its operation on February 2012 and we took 7 months for system shakedown and rapid development of its important target applications including QCD, Astrophysics and Bioscience at CCS. Then HA-PACS Base Cluster has been opened for public use from October 2012 under the Collaborative Interdisciplinary Program by CCS. 100% of system resources are dedicated for this program.

HA-PACS Base Cluster finished its operation on March 2018. Through the entire operation, the system was almost stable except the intermittent failure of GPU because of its very high density packaging in the chassis. A computation node of HA-PACS Base Cluster was one of the most advanced packaging under normal air cooling to gather two sockets of high performance CPUs and four cards of high-end GPUs as well as two channel of InfiniBand HCA. We carefully designed the air flow inside the chassis but the average temperature of each GPU is relatively high, especially for two of them located at the bottom part of motherboard where the cooling air is hot. However in average, we counted approximately 3 or 4 GPUs failure out of 1072 of them in the system on every month. Thanks to the feature of flat configuration with 268 computation nodes and full-bisection bandwidth of Fat-Tree network, the freedom of node allocation and scheduling is very high and the high utilization ratio with more than 70% in average has been kept.

HA-PACS/TCA started its operation from November 2013 and ended the life time on September 2018. The development of TCA (PEACH2) brought us a valuable experience on FPGA-base inter-GPU communication feature as well as the partial offloading function of FPGA from CPU. It was a unique research platform in the world to combine GPU and FPGA in the same node. Our successful research on this unique platform leaded us to the next project Cygnus to introduce more aggressive use of FPGA with GPU.

5.2 JCAHPC and Oakforest-PACS Project

Motivation and Objective

In 2013, The Center for Computational Sciences (CCS) established the "Joint Center for Advanced High Performance Computing (JCAHPC)" in order to design, develop, operate and manage a world-leading supercomputer system jointly with the Information Technology Center (ITC) at the University of Tokyo. Establishing the joint supercomputer center was an ambitious attempt in Japan, but it was required to install and operate a leadership supercomputer in the world that was not possible by a single institution. JCAHPC also designs and develops the core system software including operating system, programming language, and numerical libraries in collaboration with other related institutions. JCAHPC introduced Oakforest-PACS in 2016, which was the fastest supercomputer in Japan. JCAHPC promotes advanced computational sciences and contributes for the evolution of science and technology.

System Overview

The performance of the Oakforest-PACS exceeds the K computer at RIKEN AICS (currently R-CCS) that was the fastest supercomputer in the world in 2011 in terms of both the theoretical peak performance and the Linpack benchmark performance. It employs 8,208 of compute nodes where each node is equipped with a 68-core Intel Xeon Phi 7250 (Knights Landing architecture; peak performance is 3.05 TFlops) many-core processor, which are connected by 100Gbps Intel Omni-Path architecture in full bisection fat tree network topology. The overall system specification of the Oakforest-PACS is shown in the Table 1.

Theoretical Peak Performance	25 PFlops
Number of Compute Nodes	8,208
Memory capacity	919 TBytes
Interconnection Network	100 Gbps Omni-Path
Network Topology	Full Bisection Fat Tree
Parallel File System	26 PBytes Lustre File System
File Cache System	864 TBytes DDN IME

Table 1. Overall System Specification of Oakforest-PACS

It was the world largest Knights Landing system with the Omni-Path architecture in 2016. It also introduced 960 TBytes and 1.5 TBytes/sec of the world largest file cache system, aka a burst buffer, besides 26 PBytes parallel file system. The file cache system is an all-flush storage system to fill the performance gap between CPU and parallel file system. The Figure 1 shows an outward appearance of the Oakforest-PACS supercomputer.

Figure 1. Oakforest-PACS Supercomputer

In the Top500 list in November 2016, Oakforest-PACS ranked No. 6, which was No. 1 in Japan, with 13.55 PFlops of Linpack performance out of 25 PFlops of the theoretical peak performance. In the HPCG (High Performance Conjugate Gradient) benchmark, Oakfoset-PACS achieved 0.3855 PFlops and ranked No. 3 in November 2016. In the IO-500 list in November 2017, Oakforest-PACS ranked No. 1 using the world largest file cache system. Storage performance in supercomputers is critical for large-scale simulation, big data analysis, and artificial intelligence. The IO-500 list facilitates to improve the storage performance that greatly helps to improve the CPU performance.

CPU	1.4 GHz 68-core Intel Xeon Phi 7250
Theoretical Peak Performance	3.0464 TFlops
Memory	96 GBytes DDR4 and 16 GBytes MCDRAM

Table 2. Node Specification of the Oakforest-PACS

Table 2 shows the node specification of the Oakforest-PACS. Xeon Phi 7250 has embedded 16 GBytes MCDRAM that has more bandwidth than the 96 GBytes DDR4 main memory. MCDRAM can be used in a cache mode and a flat mode. In the cache mode, MCDRAM is transparently used as a memory cache of the DDR4 memory. In the flat mode, MCDRAM and DDR4 are different NUMA domains. Users can specify MCDRAM and/or DDR4 memories for their own usage. MCDRAM has better bandwidth than the DDR4 memory, while it has larger latency than the DDR4. There is further opportunity to optimize the memory performance. That is why we provide two kind of job queues for the cache mode and the flat mode. We started the configuration of the half compute nodes in the cache mode and the half compute nodes in the flat mode. After two years from the operation started, the node usage of the flat mode is more than that of the cache mode. We changed the ratio of two modes slightly, and increased the number of compute nodes in the flat mode.

Regarding the storage of the Oakforest-PACS, we introduced the file cache system besides the parallel file system. The theoretical peak performance of the CPU is 25 PFlops, and the total memory capacity is 919 TB including MCDRAM and DDR4. The rule of thumbs indicates we need more than 25 PBytes capacity. To store all memory data to a storage system within 10 minutes, the required I/O bandwidth is 1.5 TByte/sec. The total number of compute nodes are 8,208. File creation performance in a single directory requires more than 8,000 operations in a second, which means it takes one second to create a file using 8,000 processes. 1.5 TBytes/sec of storage bandwidth is challenging. When assuming a hard disk drive (HDD) achieves 200 Mbytes/sec of bandwidth for sequential access, it requires 7,500 HDDs to achieve 1.5 TBytes/sec. When each HDD has 6 TBytes capacity, the total capacity will be 45 PBytes that is much more than required. Issue that is more difficult is a single shared file access performance, which each process accesses a shared file but different part of it. There are several research efforts for this challenge that introduce intermediate storage layer between applications and a parallel file system. That is why we introduce an all-flush file cache system between applications and a parallel file system to achieve 1.5 TBytes/sec of storage bandwidth even in a single shared file access pattern.

	Capacity (TB)	Bandwidth (GBytes/sec)
File Cache System	864	1,560
Parallel File System	26,000	500

Table 3. Storage Specification of Oakforest-PACS

Overall storage specification of Oakforest-PACS is shown in the Table 3. The required storage capacity is provided by the parallel file system and the required I/O bandwidth is provided by the file cache system. The capacity of the file cache system is almost same as the total memory capacity. It is not considered to be enough but minimum capacity. Software for the file cache system is DDN infinite memory engine (IME), which is an intermediate layer based on a parallel log structured file system. From compute nodes, applications can access using POSIX and MPI-IO. File staging between the parallel file system and the file cache system is integrated with a batch job queuing system. There are several commands to check staging status, and also to manually stage-in, stage-out, and release files and directories.

System software research includes IHK/McKernel lightweight multi-kernel operating system, XcalableMP directive-based parallel language, ppOpen-HPC numerical library, and Gfarm distributed file system. IHK/McKernel mitigates the operating system jitter for parallel applications and improves the application performance. Development of all system software continues and they will be used by the Fugaku supercomputer, the next Japanese flagship supercomputer.

Operation

We started the full system operation of Oakforest-PACS from December 2016. Although Oakforest-PACS is a supercomputer operated by JCAHPC, CPU node hours are managed by CCS, the University of Tsukuba, and ITC, the University of Tokyo. CCS manages one-third CPU node hours by the Multidisciplinary Cooperate Research Program, the High Performance Computing Infrastructure (HPCI) Program, and the General Program.

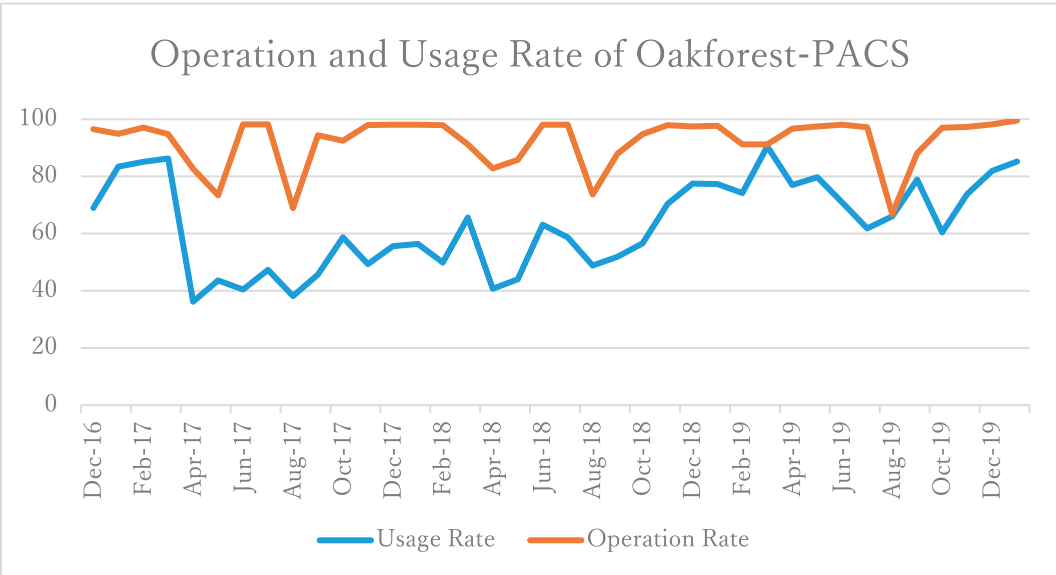


Figure 2. Operation and Usage Rate of Oakforest-PACS

Figure 2 shows the operation and usage rate of the Oakforest-PACS since December 2016. Because we cannot separate the usage by CCS programs and ITC programs, the graph shows the total usage and operation rate. From December 2016 to March 2017, it was the term for special usage for improvement of stability and performance. During this period, we found several issues of Xeon Phi 7250 and Omni-Path architecture because Oakforest-PACS was the world earliest and largest installation of them. After April 2016, the full system has been provided to all users. In August, the operation rate was dropped due to power saving in summer. The usage rate increases gradually, and it is 73.6% in average from April 2019.

5.3 Cygnus Project

Motivation and Objective

After the successful development and operation of HA-PACS/TCA System (see Section 5.1 of this part), we entered to the new phase of advanced accelerated computing. In the TCA research, we mainly introduced FPGA (Field Programmable Gate Array) for inter-GPU communication with high bandwidth and low latency of inter-node accelerating. In the final phase of research, we tried to implement a complicated computation which is not suitable for GPU into FPGA. In these days, the technology of FPGA did not allow us to implement a large scale circuit, but we confirmed that it is a very effective way to offload the calculation feature not suitable for GPU. The speed-up with FPGA for partial offloading achieved up to 7.8x performance than CPU and GPU implementation.

When we consider the next generation of accelerated supercomputers, GPU is still the main player for scientific computation even in the latter half of 2010. Actually, 6 machines in TOP10 list out of TOP500 List on November 2019 are equipped with advanced GPUs. However, we consider that GPU is not almighty because it implies several problems where it is applied to the following application characteristics:

- Low degree of parallelism in the application/algorithm: GPU is basically an SIMD device with large count of simple core elements, so that it achieves high performance when the operation parallelism reaches to several thousands per clock. However, some application reduces it partially during the computation. Due to Amdahl's Law, the inefficient computation part degrades the performance even with the state-of-the-art GPUs.
- Irregularity in computation: Since a set of computing cores (several tens in advanced one) on GPU is controlled in SIMD manner, so that the branch condition heavily degrades the computation performance. When the program encounters the condition branch, not all cores can operate and the parallelism is reduced. That causes another performance bottleneck.
- Frequent inter-GPU or inter-node communication: GPU is a slave device without interconnection feature, except recent NVIDIA GPUs equipped with NVLINK feature. General GPUs are connected to the host CPU through PCIe channel which is also shared by interconnection communication adapter such as InfiniBand HCA. When the communication is required, the control is sent back to the host CPU and internode communication is invoked. Actually communication performance is high since today's GPU is equipped with a kind of DMA over PCIe (such as GPU Direct RDMA by NVIDIA and Mellanox) to enhance the bandwidth. However, the control switching between CPU and GPU causes a large overhead with kernel invoke and return.

According to Amdahl's Law, a small fraction of performance overhead finally causes a serious bottleneck on accelerated execution where the goodness of GPU may be killed. On the other hand, recent advanced FPGA has an attractive feature to cover these issues on GPU computing:

- Since FPGA is a pipelining computation device, it is tough even for small degree of parallelism. Under the careful design of circuit, it can drive clock level pipelining can tolerate the computation performance regardless the vector length.
- Pipelining feature of FPGA computing is highly efficient even with frequent conditioning branches. The pipeline always work for any operation following to the branch, and either "if" or "else" branch can be calculated always.
- Recent advanced FPGA for HPC is equipped with direct optical communication interface up to 100Gbps of performance. It is not available on CPU nor GPU, so that it provides very low latency and high bandwidth of communication between multiple FPGAs. With careful programming, FPGA can communicate with each other without host CPU's help.

Of course, the absolute floating point performance of current FPGA is not comparable with GPU. For instance, the most advanced Intel Stratix10 FPGA can provide 10TFLOPS of theoretical peak in single precision (SP), but there is no fard-IP feature for double precision (DP) while NVIDIA Tesla V100 provides 7TFLOPS of DP performance. Therefore, we conceptually introduce both GPU and FPGA together as a "360 degree" coverage of any application feature. When GPU and FPGA work together, we can offload the computation load according to its characteristics, and also we can invoke a direct communication on FPGA. This concept is named as "Accelerator in Swtich (AiS)"

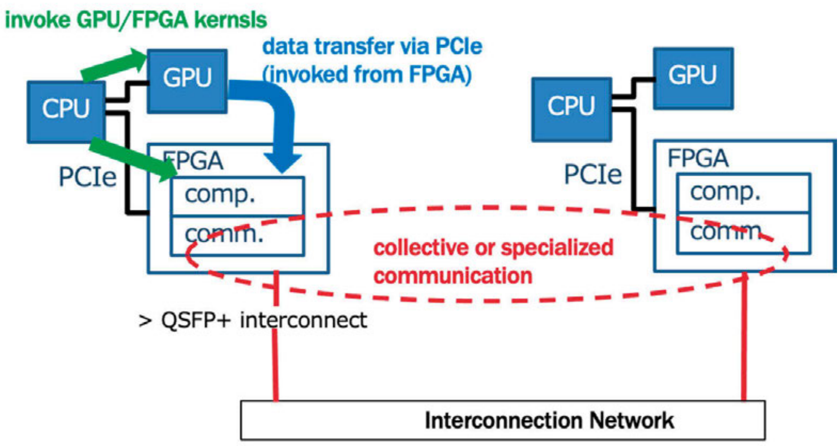


Fig.1 Accelerator in Switch where GPU and FPGA co-work

We had been researching on how to realize this concept on actual supercomputers and developing various modules on FPGA to utilize PCIe interface and optical link interface toward new generation of multi-hybrid accelerated computing from 2017. Based on our experimental prototype system named PACS-X Prototype (PPX) which is a small cluster with 12 nodes where each node is equipped with two GPU cards and one FPGA card. We also awarded with 5 years of supporting budget for system software development from MEXT ("Research and Development on Computation/Communication Unified Accelerated Computing", US$950,000 for 2018-2022). For the detailed research, see "Project Office for Exascale Computing System Development" (Section 5.7.2).

As a result after the basic research, the CCS decided to introduce a new supercomputer which is the world first real system equipped with GPU and FPGA together, named "Cygnus". The system concept is also named "Multi-Hybrid Accelerated Supercomputer" where the multiple types of accelerating devices (GPU and FPGA) are introduced. The goal of Cygnus Project is to provide a platform where these two accelerating devices work under proper application design and also the codesigning of multi-hybrid acceleration for various applications where GPU-only solution is not enough. We also aim the construction of theory and methodology for next generation of accelerated supercomputing.

System Overview

Cygnus is a cluster style of supercomputer with 80 nodes in total. A cluster with 80 nodes seem to be a small one, however each node of Cygnus is quite powerful for computation and relatively low power consuming. There are two parts in the Cygnus system where a collection of nodes with GPU and FPGA are equipped, and where the node is equipped with only GPUs. The first part is called "Albireo" and the second one is called "Deneb" according to the Beta and Alpha stars of Cygnus Constellation in the sky. There number of nodes in Albireo part and Deneb part are 32 and 48, respectively. They are connected by a fat-tree network with full bisection bandwidth.

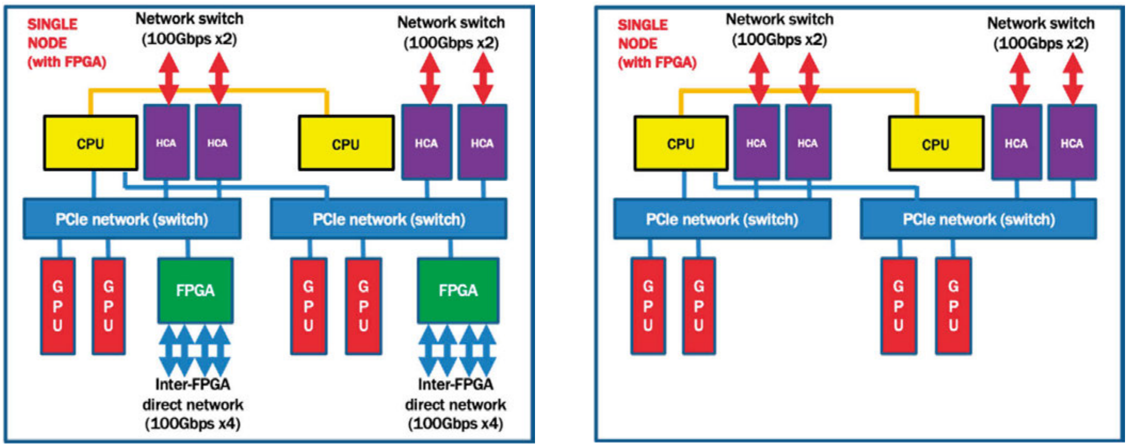


Fig. 2 Block diagram of "Albireo" node (left) and "Deneb" node (right) in Cygnus

Fig. 2 shows the block diagram of computation nodes of Cygnus. There are four GPUs (NVIDIA Tesla V100 PCIe) and two FPGAs (Intel Stratix10 with DDR and four channels of 100Gbps optical link) as well as four Mellanox InfiniBand HDR100 HCAs (100Gbps) in an Albireo node. "Deneb" node is in the same configuration with Albireo except there is no FPGA. As described before, GPU is still the most powerful device to provide absolute performance of floating point operations, and Albireo/Deneb node provides 28 TFLOPS or 56 TFLOPS of peak performance in DP or SP, respectively. To support such a high performance, we provide four cards of InfiniBand HDR100 with aggregated 400 Gbps of interconnection bandwidth. Since our main target of applications are traditional scientific computation as well as AI applications, we think the interconnection bandwidth is crucial to support large scale parallel computing. All the 80 nodes are flatly connected in fat-tree configuration for easy allocation and scheduling of nodes in batch scheduling.

Each node of Albireo and Deneb parts is also equipped with 1.6 TByte of NVMe drive as local storage for system support and advanced experiment where NVMe access over InfiniBand or control from FPGA is available. A shared file system with Lustre is equipped over InfiniBand network to be shared by all nodes. The overall specification of Cygnus is shown in Table 1.

The Lustre file system can be accessed from any node for the freedom of node allocation in any size of parallel processing. Since the system size is not quite large, only with 80 nodes, Cygnus does not introduce spine switches with large number of ports. Instead of that, the network is configured by connecting 36 port InfiniBand HDR200 switches with each other in a flat level. At each port of HDR200 switch, two links from HDR100 HCA on each node are merged so that it is effective to combine four links from a node are connected to two ports at the switch.

Table 1 Specification of Cygnus System

Item	Specification
Peak performance	2.4 PFLOPS DP (GPU: 2.24 PFLOPS, CPU: 0.16 PFLOPS + FPGA: 0.64 SP FLOPS)
# of nodes	80 (32 Albireo nodes, 48 Deneb nodes)
CPU / node	Intel Xeon Gold x2 sockets
GPU / node	NVIDIA Tesla V100 x4 (PCIe)
FPGA / node	Nallatech (Bittware) 520N with Intel Stratix10 x2 (each with 100Gbps x4 links)
NVMe	Intel NVMe 1.6TB, driven by NVMe-oF Target Offload
Global File System	DDN Lustre, RAID6, 2.5 PB
Interconnection Network	Mellanox InfiniBand HDR100 x4 = 400Gbps/node (SW=HDR200)
Total Network B/W	4 TB/s
Programming Language	CPU: C, C++, Fortran, OpenMP GPU: OpenACC, CUDA FPGA: OpenCL, Verilog HDL
MPI	MVAPICH2, IntelMPI with GDR + original FPGA-GPU-communication library
System Integrator	NEC

Fig. 3 Cygnus overlook

The name of "Cygnus" comes from its conceptual design with AiS. In the universe, there is a galaxy named "Cygnus-A" at the direction of Cygnus Constellation where two jet streams are going out. It makes us imagine the performance source with GPU and FPGA. Also, the node name "Albireo" comes from the Beta star of Cygnus Constellation where double stars configure it rotating with each other, and these double stars are symbolic for multi-hybrid acceleration by GPU and FPGA.

Another uniqueness of Cygnus is the interconnection network among FPGAs. Since each FPGA card with Intel Stratix10 is equipped with four links of 100Gbps optical connection (QSFP28), we can configure a 2-D Torus network with 8x8 FPGAs. Although the number of Albireo nodes is 32, the total number of FPGAs is 64 because there are two FPGA cards in each node. A special feature of routing function is required to utilize this 2-D Torus network, however the detail is described in Section 5.7.2. Fig. 4 shows the interconnection configuration of Cygnus with fat-tree of InfiniBand and 2-D Torus FPGA network.

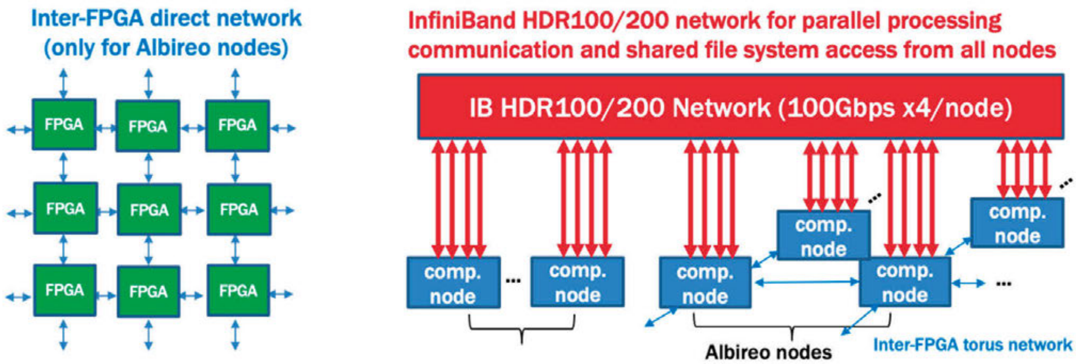


Fig. 4 Two types of interconnection network in Cygnus; fat-tree InfiniBand network and 2-D Torus (8x8) FPGA interconnection network

Operation

From April 2019, Cygnus started its operation. After one month of shake-down test, it has been generally opened for MCRP and HPCI programs to be used by nation wide researchers. Ordinary user who need GPU computing can use entire 80 nodes. Since Deneb node and Albireo node are identical except FPGA configuration, GPU-only job can run on either node. For jobs using FPGA or GPU+FPGA together, there is a special batch queue for running on Albireo nodes. The job control on FPGA is much more complicated than GPU because some users want to change the basic configuration of FPGA which is called Board Supporting Package (BSP). There is a standard BSP provided from Intel is usually configured on FPGA card, however the advanced user wants to install his own BSP, so that it must be overloaded to the FPGA board where the rebooting of FPGA is required.

The operation of Cygnus is the same as ordinary cluster systems under batch job scheduler (NEC NQSV). As in January 2020, Cygnus is mostly used by users under MCRP. When Cygnus was under procurement, the HPCI general use program had been closed on call for projects phase, and almost no project applied to use Cygnus. We will have more users on HPCI program in FY2020.

After 9 months of operation of Cygnus, the GPU utilization has no problem while FPGA utilization caused several problems. Especially for BSP rewriting on FPGA causes unstability on the nodes. We have updated the operating system and farmware of CPU to tolerate the problem. It is fixed recently. The total utilization rate of Cygnus is around 40% only. Many users still consider the system as testing platform for their new GPU- or FPGA-ready applications. We expect higher utilization rate in FY2020.

5.4 ILDG/JLDG project

Overview

JLDG (Japan Lattice Data Grid) is a data-grid for lattice QCD (LQCD) research community in Japan. See Figure 1 for a schematic diagram of the JLDG together with related systems. File servers installed on major LQCD research sites are connected to the NII (National Institute of Informatics) SINET VPN, called HEPnet-J/sc and bound into a Unix-like filesystem without partition boundary by a grid filesystem software GFarm. Using the filesystem, which looks the same from any sites, research groups can manage their data generated with several supercomputers installed at different sites and share research data within the collaboration; e.g. users can calculate physical quantities on QCD ensembles generated at a different site.

System development of the JLDG begun in 2005 and official operation started in 2008. After a key improvement of FUSE mount of the JLDG filesystem in 2011 and developments of subsystems, ILDG gateway in 2009 and a cooperative system with the HPCI in 2013, both

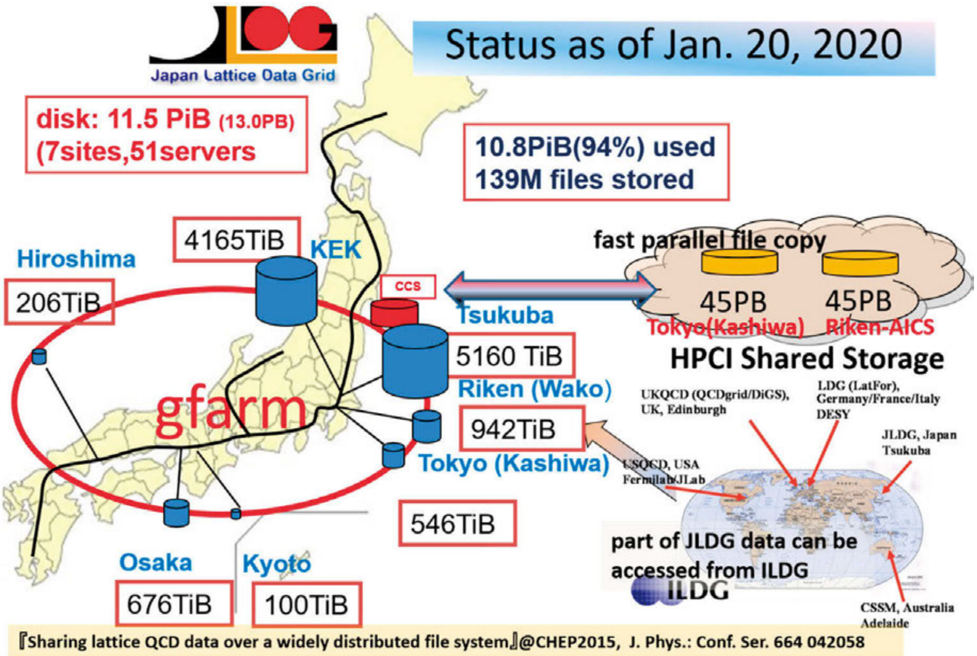


Figure 1. JLDG and related systems ILDG and HPCI Shared Storage.

explained below, the JLDG continues stable operation. As of January 2020, 16 research groups with 114 users share daily research data of 139 Million files using 13PB JLDG disk space. In January 2014, figures were; 11 groups, 67 users, 57 Million files, 2.4PB.

Although the JLDG is a joint project of participating universities and institutes, and the admin team consists of representatives of the JLDG sites and research groups, it has been continuously led by the CCS, mainly because experts from three divisions get together and work in the collaboration; we have a developer of the Gfarm from “Division of High Performance Computer Systems”, an expert of database from “Division of Computational Informatics” and a staff from “Division of Particle Physics” who knows needs of LQCD researchers.

On the other hand, ILDG is a worldwide grid of 5 regional data-grids for sharing LQCD configurations through the common interface of exchanging metadata and data or ensembles and configurations. The CCS worked as a representative of the Japanese grid and contributed to the ILDG in various ways. JLDG subsystem to provide ILDG users with public data was developed in 2008 and faceted navigation system, a search interface of ensembles in 2009. Members of the CCS took the role of the ILDG board and metadata and middleware working group members (chair/convener for some time). And above all, the CCS provides 53 public ensembles (33000 configurations).

Another subsystem enables us to copy files in multiple streams between the JLDG and the HPCI Shared Storage, where the HPCI is a Japanese national project started in 2011 for constructing High Performance Computing Infrastructure. The subsystem was constructed in 2013 and started its operation in 2014. The benefit of the subsystem is high for LQCD projects approved by the HPCI.

Activities

In 2014, the JLDG was working as an infrastructure for researchers in LQCD community. Hence activities for the next 6 years shifted to upgrade and maintenance of system hardware and software. Among these, important updates are as follows.

1. <u>Reorganization of JLDG sites.</u> Two new sites, the YITP of Kyoto University and the RIKEN Nishina Center, joined the JLDG in 2014. The YITP, a research center, open to theoretical physicists in Japan, brought new users and the RIKEN provides storage systems as well. On the other hand, the KMI of Nagoya University and Kanazawa University were disconnected in 2016, mainly because staff working for the JLDG moved to other institutes. In 2018, the University of Tokyo site is reorganized to have JLDG specific file servers. Before then, the JLDG borrowed disk space from the HPCI.

   We plan to start a new site at Riken Center for Computational Science (R-CCS) very soon. Formal procedures and installation of facilities have already been completed. The new supercomputer Fugaku, a successor of the K computer, is expected to connect to the JLDG as a client.

2. Filesystem software update. As the first practical grid file system of the Gfarm, we often give feedback to the Gfarm for improvement. "Checksum on the fly" implemented in 2014 and its improved version in 2016 drastically improve solidness against data loss or corruption. A checksum (md5sum) is calculated at each file/replica read/write and is stored in the MDC or compared with the stored value. In addition, after 6 hours of file (replica) creation, the file is read again to calculate and check the checksum. The latter enables us to detect e.g. data transmission error and temporal filesystem error, while the former, the so-called silent data corruption. Checksum mismatch really happens in the JLDG, though frequency is not high, we could recover data from replicas for all cases and hence user had no damage of losing valuable data.

Item	Value (ratio)	population	
Total I/O	630 TiB (17%)	Total Data	3704 TiB
Write (upload)	435 TiB (69%)	Total I/O	630 TiB
Read (download)	195 TiB (31%)	Total I/O	630 TiB
# I/O files	23.1 M (17%)	# files	139 M
# I/O users	35 (42%)	#reg users	114+23
# used clients	21		

Figure 2. Statistics Jan.2019 -- Dec.2019

3. Updates of supporting servers and network. The JLDG needs several servers to control the JLDG filesystem. Both hardware and software of these servers are updated several times. a) A slave metadata server was installed at the RCNP of Osaka University in 2014. When the CCS, Tsukuba is down due to scheduled power cut, we continue operation of the JLDG using the slave server and file servers outside the CCS. b) A monitoring system was reconstructed using Zabbix software in 2014. c) Following an update of the backbone NII network from SINET4 to SINET5 in 2015, we have installed several 10Gbps switches for the JLDG site local network. Many file servers installed at several sites are now connected via 10Gbps networks instead of previous 1Gbps networks. d) Several servers, which had been physical machines, were put together into two server machines using KVM virtualization technology in 2016. e) The cooperation subsystem with HPCI-SS, which was developed in 2013 and started its operation in 2014, was improved in 2016: Symbolic link of the Gfarm was applied to the HPCI-SS file system. f) A remote maintenance system was developed using intel AMT technology and was installed at the Univ. of Tokyo site in 2018. The system enables us to control servers (including power on/off and operations using console), an UPS and a network switch from the CCS. Such a system is required because no full-time staff can take care of

the JLDG site. g) In 2018, we wrote a set of scripts to summarize the utilization information during a specified period, such as I/O (read and write) in Terabytes, the number of accessed files and the number of active users. See Figure 2 for an example of results. h) IPMI network was constructed for the CCS servers in 2019.

4. Continuous installation of new file servers. We have increased the capacity of the JLDG file system by installing new file servers every year. As of January 2014, we had a disk space of 2.4PB constructed over 20 servers. Disk space (number of servers) at the beginning of each year was 5.0PB(28) in 2015, 7.5PB(39) in 2016, 9.0PB(43) in 2017, 11.1PB(47) in 2018, 12.4PB(49) in 2019 and 13.0PB(51) in 2020. For a reference, we reproduce disk space used for files and replicas in Figure 3.

Although each activity is not conspicuous, activities in total improve the availability of the JLDG. In addition to productive and visible works described above, works to maintain and improve the security of the JLDG and ILDG increase, and account for the large portion of work time, especially in recent years. We review and improve security settings such as network switch ACL and firewall of individual servers, manage vulnerabilities and analyze security logs.

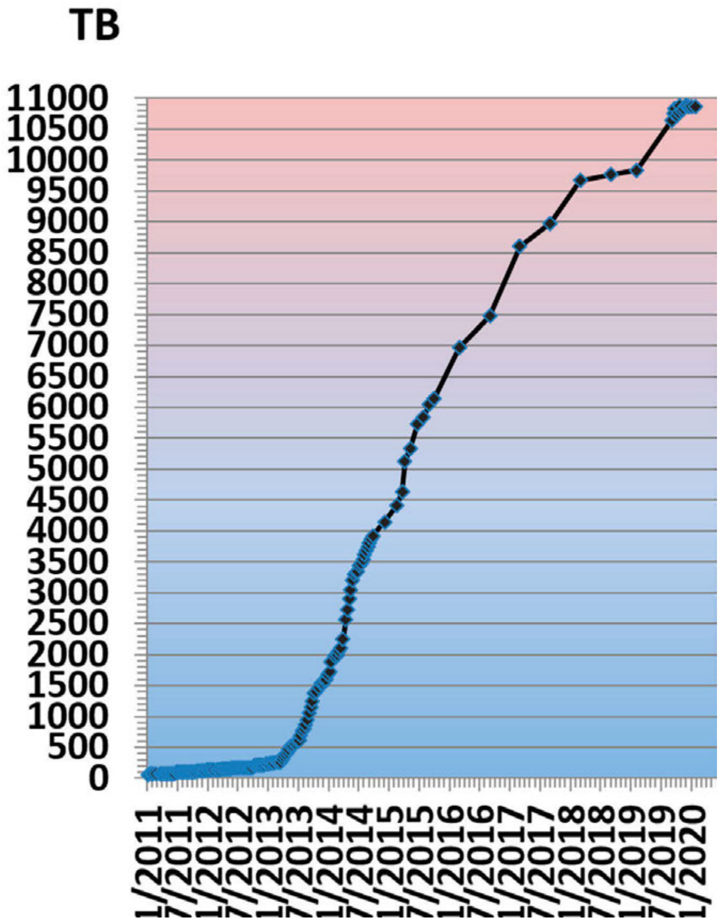


Figure 3. Disk space used for files and replicas.

Activities related to the ILDG project are summarized as follows.

1. Maintaining the ILDG interface. The official ILDG interface consists of Metadata Catalog (MDC) Service and File Catalog (FC) Service. Unfortunately, it turns out that the web service software package we use for the JLDG MDC has security vulnerabilities and an update of the package was difficult to keep compatibilities. Therefore, we suspended the MDC service in July 2018. Instead, we provide the community with a workaround: faceted navigation system developed at the CCS substitutes functions of the MDC; it gives us Markov Chain URI of an ensemble and a set of LFNs of configurations. We present a conversion program from LFN to TURI to the public, which is a function of the FC: LFN to TURI is one-to-one mapping for the JLDG.
2. Access to JLDG public data. JLDG keeps 59 ensembles (39000 configurations) generated by five physics projects. These data have been kept public to the LQCD community. ILDG connections, mainly made from abroad, counted 3200 for 6 years and downloaded 15600 configurations. Note that Japanese colleagues can access public data via the JLDG interface which is much easier to use than the ILDG interface. We don't record access of this type because it is difficult to distinguish access to public data and that to private data. Unfortunately, we have not published new data. We are preparing 2+1 flavor QCD configurations generated with the K computer on a 96^4 lattice at the physical point of u/d quark masses.
3. DOI assignment to QCD ensembles. The DOI (Digital Object Identifier) plays a key role ensuring long term access to digital data. DOI has been assigned to scientific publications. Assigning DOI to research data is becoming standard, partly because researchers can cite the DOI of data they used as references. It is usual that the number of citations of a paper is regarded as a measure of the superiority of the paper, and it will be similar for research data. Therefore, assigning a DOI to research data encourages researchers to publish data themselves. It also gives us a method to track how published data are used. Assigning DOI to QCD ensembles is pioneered by the USQCD and a demonstration is given at the ILDG 23rd, a video workshop in April 2015. Some of JLDG members were inspired by the presentation and have been working to establish a framework of DOI assigning to JLDG QCD ensembles. As of January 2020, the DOI working group of the JLDG team finalized "terms and agreements" and "procedures" of DOI assignment. They are approved by the JICFuS (Joint Institute for Computational Fundamental Sciences) and the CCS is approved as a member of JaLC (Japan Link Center). Tools have also been completed to generate a landing page of QCD ensemble from an ILDG QCDml XML of the ensemble. We will do the first assignment of DOI to a JLDG public QCD ensemble.

There are several problems/issues to be solved. We list them as concluding remarks.

1. Some basic software supporting the JLDG is becoming obsolete, e.g., the Globus toolkit retired in 2018.
2. Reconsideration of operation policy of the JLDG, such as “no quota for no charge”.
3. Reconsideration of QCD data sharing worldwide. ILDG activity is not high in the last several years. We may reactivate the ILDG or look for another framework if necessary.
4. Plan to ensure that the necessary budgets and staff are secured.

5.5 Multidisciplinary Cooperative Research Program

A mission of the CCS is promoting research activities in computational sciences worldwide. The CCS scientists consist of those in a variety of fields. They not only utilize computers for their own research purposes, but also work in close collaboration with computer scientists to develop and design novel computers that are most suitable for various scientific applications. Since 2002, the Center has been making computer resources available to collaborative research projects in order to facilitate nationwide progress in computational sciences. Since 2007, these activities have been reinforced by enhanced links with computer sciences through the promotion of the Multidisciplinary Cooperative Research Program (MCRP). Since 2010, the CCS has been recognized as a national core-center under the Advanced Interdisciplinary Computational Science Collaboration Initiative (AISCI). The MCRP has been open to overseas researchers as well, however, the project leaders must have been affiliated in institutes in Japan. This restriction has been lifted since 2019. Now, the MCRP proposals can be directly submitted from abroad. The MCRP is also providing cooperative assistance and supporting research meetings, visitors, travels, and short-term employment for cooperative researches in various fields.

The CCS has been accepting proposals for the MCRP in many fields of computational sciences, including particle and nuclear physics, astrophysics, material sciences, life sciences, global environmental sciences, biology, and chemistry, as well as in the fields of computer sciences including high performance computer systems, computational informatics, and numerical analysis. The submitted proposals are reviewed and approved/rejected by Cooperative Research Committee which consists of two (one) committees from outside (inside) University of Tsukuba in each field. The MCRP projects are provided with the approved amount of CPU time of free use in supercomputers operated by the CCS. Computational facilities provided by MCRP include HA-PACS/TCA [Highly Accelerated Parallel Advanced system for Computational Sciences] (2013-2018; 64 nodes, 364 Tflops), COMA [Cluster Of Many-core Architecture processor] (2014-2019; 393 nodes, 1 Pflops), Oakforest-PACS (2017-Present; 8208 nodes, 25 Pflops), and Cygnus (2019-Present; 80 nodes, 2.4 Pflops). In 2018, we have launched an online submission system of the proposals. Then, in 2019, the language of the online system has been switched into English and open worldwide.

The number of MCRP-approved projects conducted over the last six years is shown in Table 1. Approximately forty to eighty projects are approved each year, and the number is steadily increasing. This clearly shows large needs of our societies for resources of high-performance computing. The CCS has been and will be contributing to these demands in various fields of science. We also show in Figure 1 the ratio of the number of MCRP projects in each field, approved in 2019. This demonstrates that we have the MCRP projects across a variety fields of natural science and engineering. In fact, the MCRP helps researchers to produce a significant number of publications every year, for instance, 229 (263) publications in international journals in 2018 (2017).

We organize a symposium in October every year, to give researchers in the computational sciences a nice opportunity to interact with those with many different disciplines. The symposium consists of keynote and invited talks in a variety of fields of computational sciences, and of poster presentations as the MCRP reports. The official language of the symposium was Japanese but switched to English since 2018. They are listed below.

Table 1: Number of approved projects in MCRP.

Year	# of projects	Computers
FY2019	78	Oakforest-PACS, Cygnus
FY2018	67	COMA, Oakforest-PACS
FY2017	61	HA-PACS, COMA, Oakforest-PACS
FY2016	62	HA-PACS, COMA
FY2015	51	HA-PACS, COMA
FY2014	41	HA-PACS, COMA

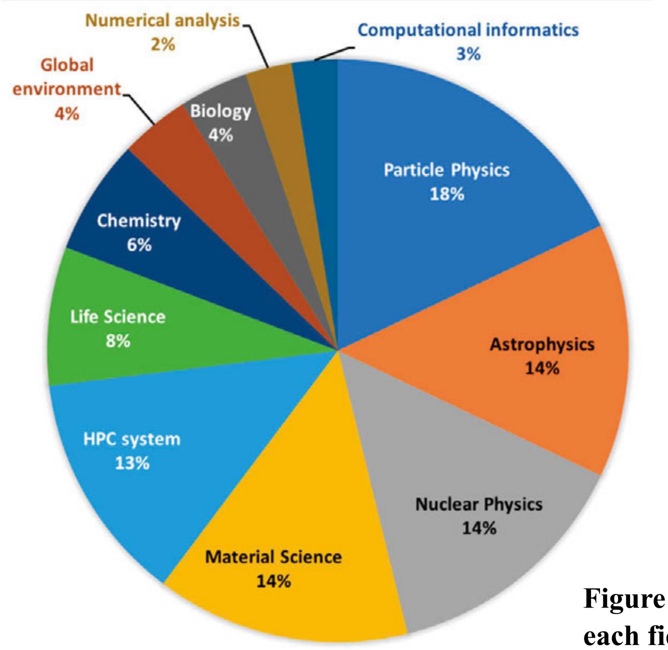


Figure 1: Ratio of number of proposals in each field (MCRP-2019)

Symposiums Organized by the CCS since 2014

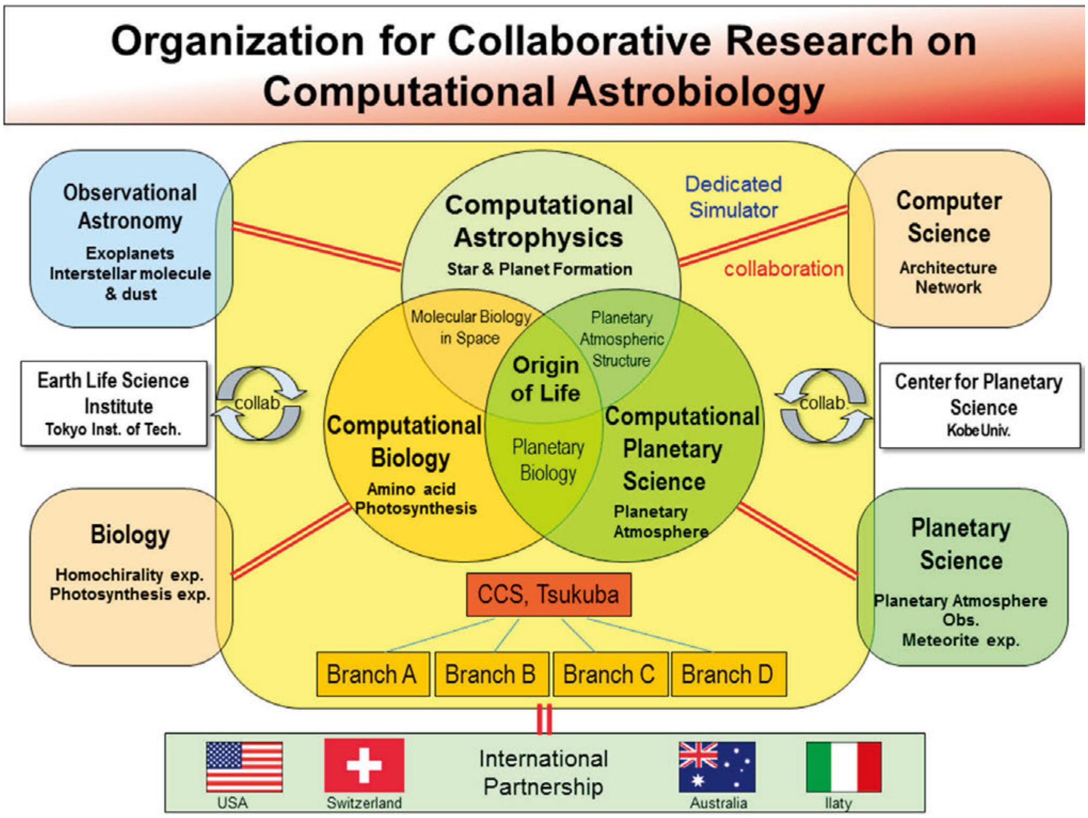
- 11th symposium on “Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences”, Oct. 15, 2019, Tsukuba Int. Congress Center
- 10th symposium on “Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences”, Oct. 15-16, 2018, University of Tsukuba
- The 25th Anniversary Memorial Symposium of CCS, Univ. Tsukuba “Progress and Future of Computational Sciences” and 9th symposium on “Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences”, Oct. 10-11, 2017, Tsukuba Int. Congress Center
- 8th symposium on “Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences”, Oct. 17-18, 2016, University of Tsukuba
- 7th symposium on “Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences”, Oct. 19-20, 2015, University of Tsukuba
- 6th symposium on “Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences”, Oct. 21-22, 2014, University of Tsukuba

Figure 2: The 25th Anniversary Memorial Symposium of CCS, Univ. Tsukuba “Progress and Future of Computational Sciences” and 9th symposium on “Discovery, Fusion, Creation of New Knowledge by Multidisciplinary Computational Sciences”

5.6 Computational Astrobiology (CAB)

(by Divisions of Astrophysics & Life Sciences)

We have initiated "Organization for Computational Astrobiology". Astrobiology has attracted a significant deal of attention owing to advanced observations of extrasolar planets as well as interstellar molecules. This organization aims at exploring key processes related to the origin of life in the universe through *ab initio* calculations based on collaboration among the Computational Astrophysics, Computational Biology, and Computational Planetary Science. At present, 54 researchers from 22 institutes are participating in the organization, which was formed at the initiative of the CCS, University of Tsukuba.



These research efforts are targeted on the study of interstellar molecular biology, planetary biology, and planet formation. So far, we have worked on

- Dust growth in a turbulent protoplanetary disk
- Formation of organic molecules in interstellar space
- Cosmic origin of homochirality of amino acids

(see the reports in Divisions of Astrophysics & Life Sciences for the details). Also, in this collaboration, we have pursued a project in Exploratory Challenge on Post-K computer' (Elucidation of the Birth of Exoplanets [Second Earth] and the Environmental Variations of Planets in the Solar System).

5.7 Research Project Offices

5.7.1 Project Office for Exascale Computational Sciences

Supported by the dramatic growth of computer power, the Computational Sciences have seen remarkable developments in recent years, and are now recognized – along with theory, experiment, and observation – as indispensable partners in the promotion of the cutting-edge scientific frontiers of the 21st century.

Nowadays, computers characterized by a new architecture are appearing in rapid succession and include large-scale systems equipped with Graphics Processing Units (GPUs) as accelerators, massively-parallel computers equipped with many-core processors, which may play a central role in future large-scale computing, to say nothing of ordinary massively-parallel computers combining a multitude of central processing units (CPUs). Due to advances in such diverse computers, it becomes a difficult task for researchers to make computations with the full power of each machine.

By means of close collaborations among researchers of physics and those of computer sciences, the Center for Computational Science (CCS) has successfully achieved a number of breakthroughs by developing optimum computers for computational sciences in the fields of particle and astrophysics. Furthermore, the Center now has a Project Office for Exascale Computational Sciences dedicated to close collaborations among computational and computer scientists in a wide variety of fields, and to establishing cooperation among researchers belonging to divergent scientific fields.

The services of this Office are not restricted to the Center alone, but extend outside to promote nationwide collaborations. To date, it has conducted analyses and examinations of hot spots for major applications to ensure that they show high efficiency in Oakforest-PACS in Joint Center for Advanced High Performance Computing (JCAHPC), one of the fastest supercomputers in Japan equipped with processors of Many Integrated Core architecture, under close cooperation with the Project Office for Exascale Computing System Development, which is the organization promoting the development of new computers. Currently, developments and adjustments of computer codes that run efficiently at Cygnus, equipped with both GPU and field-programmable gate array (FPGA), have been a central issue at the Office. We also exchange ideas and knowledge for efficient use of Fugaku supercomputer that is planned to be soon installed at the RIKEN Center for Computational Sciences.

Activities on Oakforest-PACS undertaken by the Project Office for Exascale Computational Sciences

Field	Scientific Target	Numerical Calculations employing many-core processor
Particle Physics	•High precision calculations of the standard model of particle physics •Multiscale physics •Physics at finite temperature and density •Physics beyond the standard model	•Iterative solver for linear equations with large sparse matrices •Dense matrix-matrix multiplication •Extraction of eigenvalues and singular values
Astrophysics	•Exploring the formation of the first generation of astrophysical objects in the early universe •Exploring the structure formation of galaxies, galaxy clusters, and the large-scale structures in the universe	•Radiation transfer and radiation hydrodynamic simulations using ray-tracing method •Vlasov simulation in 6 dimensional phase space
Nuclear Physics	•Exploring many-nucleon dynamics based on unified description of nuclear structure and reactions	•Projection and configuration-mixing calculation •Time-dependent density functional theory calculations incorporating pair condensation
Material Science	•Exploring light-matter interactions and ultrafast electron dynamics in matters	•Time-dependent density functional theory calculations in real time and real space
Life Science	•Analyses of enzymatic reaction in living body •Large-scale phylogenetic analyses of eucaryote	•Fragmented molecular orbital method •Real space Car-Parrinello molecular dynamics method
Global Environmental Science	•Exploring arctic oscillation •Exploring urban climate and local wind	•Efficient solution of Poisson equation •Similarity retrieval of high-dimensional data
Computational Informatics	•Information management and knowledge discovery in massive scientific data	•Efficient processing of large graph •Cluster analysis over large-scale scientific data
Mathematical modeling and algorithms	•Large-scale parallel computational methods in computational sciences	•Parallel algorithms for a generalized eigenvalue problem of dense matrices •Development of eigenvalue calculation software for sparse matrices − z-Pares, CISS

5.7.2 Project office for exascale computing system development

Under codesigning manner of supercomputer development and application software implementation, we operate a project office named "Project Office for Exascale Computing System" mainly focusing on system development including architecture, hardware, system software and numerical library. The office was established during HA-PACS Project and the main job was the design and implementation of TCA (PEACH2) board for HA-PACS/TCA (see Section 5.1). Through the experience of TCA development, we reached to a concept of "multi-hybrid accelerating system" toward very high sustained performance where ordinary GPU computing is not a perfect solution. One of the trial to use FPGA (Field Programmable Gate Array) in TCA board not only for GPU-GPU communication but also for partial offloading of computing load was LET (Least Essential Tree) computing required in astrophysics simulation.

In 2016, we launched a new project named "PACS-X" for a basic technology research on multi-hybrid accelerated computing where we introduce two devices for computation offloading; GPU and FPGA. We had a research budget support from MEXT under the name of "Creation of Multidisciplinary Computational Sciences by Next Generation Computing Technology" with a budget of approximately US$1.2M in total for five years. This budget is not for building the practical machine but for fundamental research and prototype development of multi-hybrid accelerated supercomputer. Additionally, we the CCS was also awarded with a strategic competitive budget in the program of "Program for High Performance General Purpose Supercomputer Utilization" by MEXT, with the name of "Research and Development of Next Generation Computation and Communication Unified Supercomputer" (PI: Taisuke Boku) with approximately US$1M in total for five years. This is also not to build a real system for product run, but mainly focuses on the system software and typical application development under the concept of AiS. Under the support of these budget, we developed all the supporting system software, basic algorithm, mechanism combining GPU and FPGA, etc. We developed a prototype system of PACS-X as the 10th generation of our convention for the supercomputer series in the CCS. Finally, University of Tsukuba decided to introduce a multi-hybrid accelerated supercomputer with 80 nodes, 320 GPUs and 64 FPGAs at the CCS, which is named Cygnus (see Section 5.3).

Here, we introduce the core technologies of multi-hybrid accelerated supercomputing realized in Cygnus.

A. Prototype of PACS-X: PPX

We believe it was the world first attempt to combine GPU and FPGA together in a single computation node because there are a number of challenges to build, program and operate such a complicated system. However, the advanced technology for FPGA to be used for HPC rapidly became available, and we had some level of verification to realize this concept as actual machine.

Before building the actual system, we implemented a prototype system in small size with small configuration. This is a mini-cluster for proof of concept of AiS (Accelerator in Switch) to combine GPU and FPGA in a single system. It is named PPX (Pre-PACS-X). Figure 1 shows a schematic view of AiS concept.

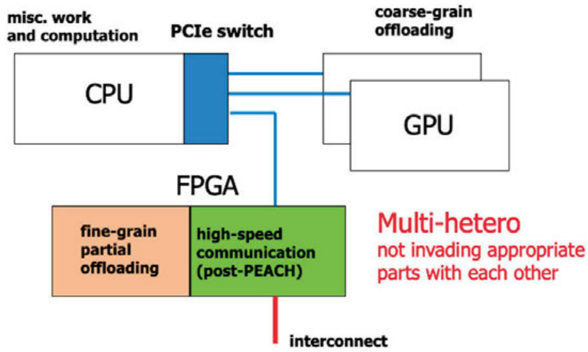


Fig.1 Concept of AiS (Accelerator in Switch)

In AiS, we introduce multiple types of accelerators such as GPU and FPGA. In the PPX phase-1 system built in 2017, we developed a mini-cluster with 6 nodes where each node is equipped with Intel Xeon CPU (2 sockets), NVIDIA Tesla P100 (2 cards) and Intel Arria10 FPGA board. In 2018, we extended the system as PPX phases-2 with almost the same architecture but introducing Xilinx Kintech FPGA instead of Arria10 for comparison between two types of FPGA. The number of nodes is 7, and the total count of nodes in phase-1 and phase-2 is 13. We also modified several nodes with advanced accelerators such as NVIDIA Tesla V100 and Intel Stratix10 FPGA to evaluate the state-of-the-art accelerator technology. Fig. 2 shows the node configuration of PPX and Fig. 3 shows the network connection among FPGAs.

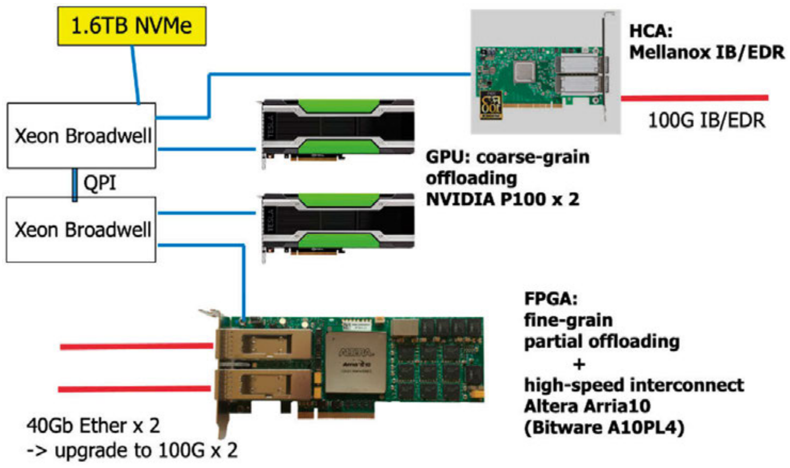


Fig. 2 PPX (phase-1) node configuration (in phase-2, FPGA is replaced with Xiling Kintech)

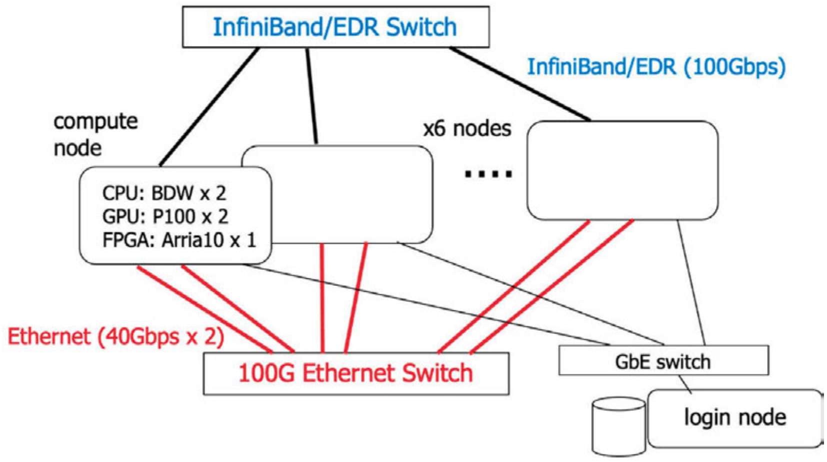


Fig. 3 Inter-node communication network of PPX (phase-1) with InfiniBand/EDR on mother board and 40Gbps optical link (2 channels) on FPGA board

When we developed PPX, we designed the inter-FPGA network to use Ethernet frame because it is quite easy to extend the system size with 40 to 100 Gbps Ethernet switch. To run the cluster as ordinary Linux one, we also provide InfiniBand/EDR HCA and switch for easy control of the system.

B. Inter-FPGA communication technology: CIRCUS

Even if a user introduces FPGA board with high speed optical link such as 40Gbps (QSFP+) or 100Gbps (QSFP28), he cannot enjoy to use it in High Level Synthesis (HLS) language such as OpenCL. The FPGA and board vendors provide a minimum set of function modules as logic IP which is available only from low level Hardware Description Language (HDL) such as Verilog HDL. Therefore, we first developed a module named Channel over Ethernet (CoE) to enable the packet send/receive through Ethernet switch and it enables us to control from OpenCL program. It is very important to prepare any programming environment of FPGA as HLS programming because no application user wants to describe HDL and we need to provide HLS environment to utilize any facility of FPGA. That is our strong policy because we like to open the system to real application users who are not familiar to FPGA programming.

CoE achieves very low latency of inter-FPGA communication driven from OpenCL user code. Fig. 4 shows the latency and bandwidth of the CoE on Intel Arria10 which has two optical link interfaces up to 40Gbps for each and is connected to the host CPU through PCIe Gen.3 x8 lanes. Here, it is shown that the CoE achieves ultra-low latency compared with traditional way of FPGA to FPGA communication through the host CPU and its InfiniBand communication with MPI. The CoE achieves less than 1us of pingpong latency (single direction) but the bandwidth is limited around 5 GByte/s because the PCIe on FPGA is not efficient even as Gen.3 x8 lanes. However, the performance curve of bandwidth rapidly raises with short message size where the low communication latency affects on the short $N_{1/2}$ of message size.

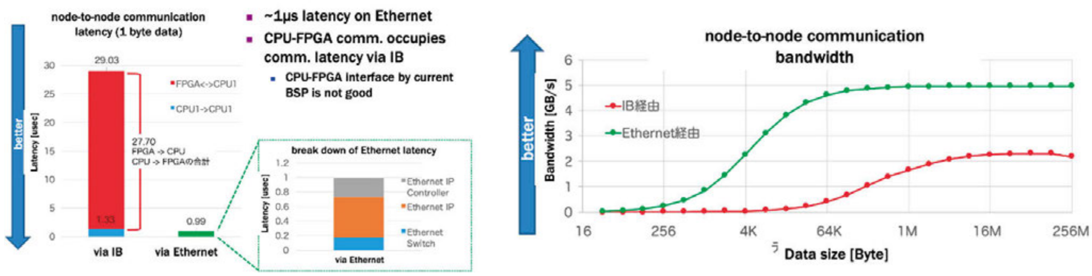
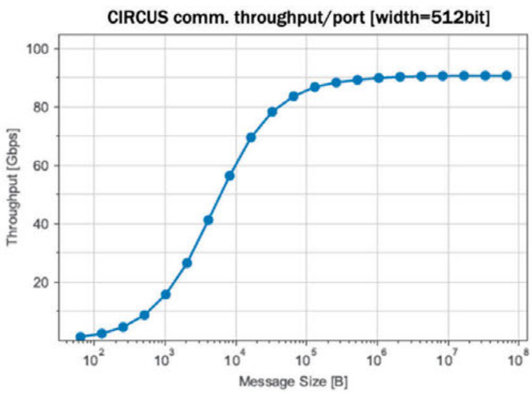


Fig. 4 Latency and bandwidth of CoE with Arria10

After development of CoE, we planned to implement it on the actual Cygnus system where an Albireo node is equipped with four NVIDIA Tesla V100 cards and two Intel Stratix10 (board is Bittware 520N) cards. Bittware 520N FPGA card is equipped with four channel of 100Gbps optical link, so that the aggregated communication performance is 5 times of Arria10. When we implemented CoE to the real Cygnus system in 2019, we decided to renew the design and implementation of CoE not to rely on the Ethernet switches to enlarge the system size. The problem we found on CoE toward implementation on Cygnus is that it depends on the packet switching with Ethernet frame and the computation on FPGA and communication by CoE cannot fully utilize the pipeline feature of FPGA. To make an Ethernet packet, we need to store the data in the communication buffer, then the message is transferred. Here, the pipeline streaming computation on FPGA circuit and message transfer are separated to break the seamless data flow. Therefore, we switched our goal to provide a "truly seamlessly combined pipelining of computation and communication". Under this concept, the computation result in the pipeline operation is transferred to the communication system with minimum chunk size (currently 512bit) and it is sent out to the optical link while the next data chunk is created by the computation. Here, we can create a truly seamless pipeline of computation/communication unification. It is available only in FPGA and different from buffering-base communication on ordinary CPU or GPU.

We named this system as Communication Integrated Reconfigurable CompUting System (CIRCUS). We implemented it on Cygnus with a routing function based on streaming data transfer. Since the inter-FPGA communication network on Cygnus is configured with 2-D Torus network (8x8) to fully utilize the four channel of 100Gbps network link (see Fig. 4 in Section 5.3), we need a routing function inside FPGA to handle the data transfer between arbitrary source/destination combination. Since we implemented everything under the policy of CIRCUS, the application user can enjoy the seamlessly pipelined computation/communication unification between any node combination for parallel processing. Fig. 5 shows the bandwidth of pingpong communication and the performance shift when multiple hops are required to transfer the data through routing feature of CIRCUS.

We are currently developing the first application based on CIRCUS with astrophysics simulation by radiative transfer for early universe object creation.



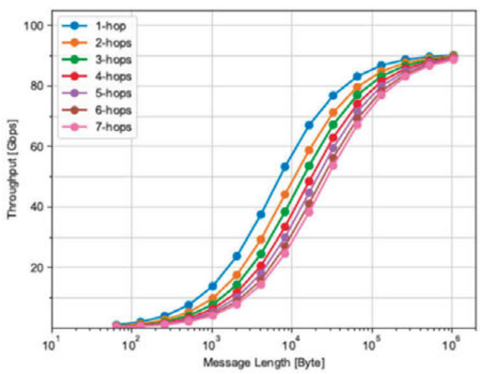


Fig.5 Bandwitdh of CIRCUS on Cygnus with direct neighboring pingpong (left) and multi-hop routing (right)

C. GPU-FPGA DMA function

Another technical issue on multi-hybrid acceleration with GPU and FPGA is how to transfer the data between these devices. Since all these devices in Cygnus are connected by PCIe Gen.3, it is theoretically possible to perform over PCIe DMA feature. It is possible to exchange the data through memory copy on the host CPU, but it is inefficient to degrade the high performance of multiple accelerators.

Basic DMA engine on PCIe bus for FPGA is provided as an IP from vendors, however we need to know how to map the object memory address on remote device to the PCIe address space. Only the host CPU knows the physical address of the variable on global memory of GPU device via CUDA API for NVIDIA GPU. So that we can get the target physical address on GPU device and it can be mapped on PCIe address space. Finally, the FPGA can control and invoke the DMA transfer between FPGA and GPU. Figure 6 shows the schematic view of DMA between GPU and FPGA (left) and address mapping information handling (right).

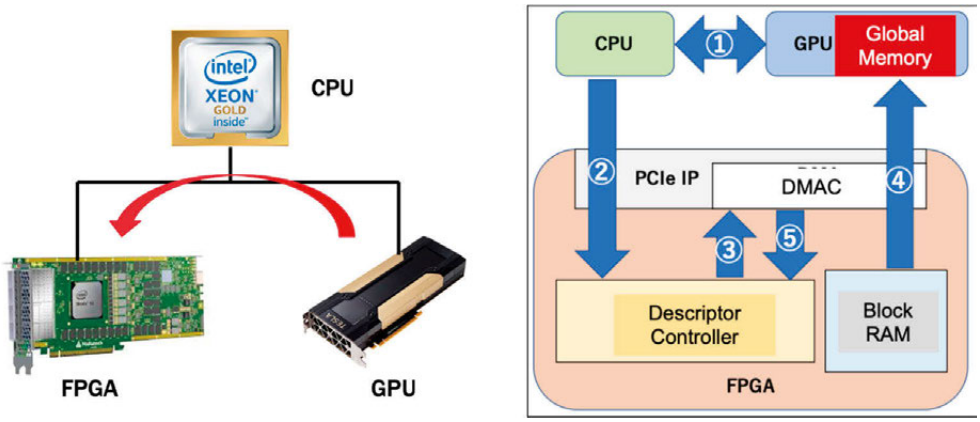


Fig. 6 DMA over PCIe between GPU and FPGA (left) and how to get the address information on GPU global memory into FPGA (right)

As same as described in the previous section, our goal is to provide an easy environment to program the FPGA control for application users, then it is required to control this flow on HLS such as OpenCL. We implemented the API feature for that on Arria10 FPGA toward final implementation on Startix10 in Cygnus. Fig. 7 shows the bandwidth of our DMA compared with the conventional data copy through the host CPU where both direction of data copy is performed via memory copy to/from the CPU memory. Here our DMA feature achieves up to 7 GByte/s and 4 GByte/s of sustained performance on FPGA-to-GPU and GPU-to-FPGA DMA transfers, respectively. These low performance lines are by CPU memory copy where the achievable results are the same with GPU-to-FPGA data copy, however the bandwidth with DMA rapidly rises even for a couple of KByte of data. Especially, the minimum latency to perform the DMA transfer is quite short where that for FPGA-to-GPU transfer is around 600nsec and the opposite direction takes 1.44usec while conventional method through CPU memory copy takes 20usec and 17usec, respectively. This improvement on latency is approximately 11x to 33x times shorter than conventional way. Such a latency-aware implementation works very efficiently when we consider the strong scaling of parallel execution.

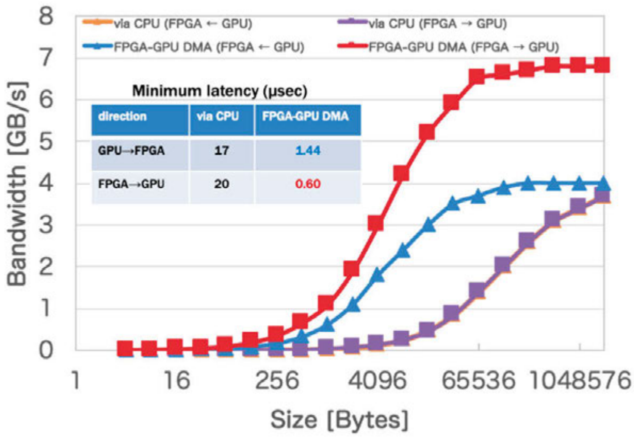


Fig. 7 DMA transfer on FPGA and performance comparison with conventional way (through CPU memory)

We design and implement such fundamental functions and methodology in Project Office for Exascale Computing System Development to support the application users to use this world most advanced system with multi-hybrid accelerating in relatively easy manner.

5.7.3 Project Office for HPCI (JICFuS)

■ HPCI Plan and Strategic Program Field 5

The innovative High Performance Computing Infrastructure (HPCI) plan, which was established with the "K computer" at the core, was created to actualize an innovative computational environment capable of meeting diverse users needs, and aimed at promoting the exploitation of HPCI. As major policy objectives, building an organization for promoting computational sciences in major fields (HPCI Strategic Program), and producing revolutionary results through the exploitation of HPCI are cited.

In the HPCI Strategic Program, which had been operated from FY2011 to FY2015, five potential fields were identified as strategic fields that not only required K computer resources, but also were expected to yield significant social and scholarly breakthroughs. "Field 5: The origin of matter and the Universe" was one of these. This field dealt with fundamental physics, primarily concerning elementary particles, the atomic nucleus, and astrophysics. The institution (strategic institution) that successfully led Field 5 research and development for five years was the Joint Institute for Computational Fundamental Science (JICFuS), which was originally founded as a joint research organization combining Center for Computational Sciences (CCS) in University of Tsukuba, the High Energy Accelerator Research Organization (KEK), and the National Astronomical Observatory of Japan (NAOJ). In 2014 JICFuS was expanded including five more research organizations (Yukawa Institute for Theoretical Physics (YITP) in Kyoto University, Research Center for Nuclear Physics (RCNP) in Osaka University, Center for Nuclear Study (CNS) in the University of Tokyo, International Center for Hadron Astrophysics (ICEHAP) in Chiba University, and RIKEN Nishina Center).

Figure 1 K computer

■ Toward the New Supercomputer "Fugaku"

The post-K computer development plan under the FLAGSHIP 2020 Project, initiated by the Ministry of Education, Culture, Sports, Science and Technology in 2014, has set the target of developing (1) the next generation flagship supercomputer of Japan (the successor of the K computer) along with (2) a wide range of applications that will address top 9 priority social and scientific issues. "Priority Issue 9: Elucidation of the fundamental laws and evolution of the universe" led by the CCS, University of Tsukuba and 10 other institutions is essentially the successor of "Field 5: The origin of matter and the Universe" aiming at new developments. The CCS also joins "Priority Issue 7: Creation of new functional devices and high-performance materials to support next-generation industries (CDMSI)". In addition to the priority issues, there are four exploratory challenges selected to be tackled using the post-K computer. The CCS joins two of them: "Exploratory Challenge 1: Frontiers of basic science: Challenging the limits" and "Exploratory Challenge 3: Elucidation of the birth of exoplanets (second earth) and the environmental variations of planets in the solar system". In May 2019 the post-K computer was officially named "Fugaku", which is another name of Mt. Fuji. The K computer was shut down at the end of August, 2019. The new supercomputer is now under installation after disassembling the K computer. The four-year project of 9 priority issues and 4 exploratory challenges will end in March of 2020. The successive projects, which focus on producing the scientific results by using Fugaku, are supposed to be operated for the next three years. The HPCI project office promotes and supports the accomplishment of research targets in the next projects.

5.7.4 Project office for AI & big data

Recently, big data and AI have attracted a great deal of public attention. In big data analysis, we analyze a massive amount of complex data that cannot be processed by ordinary computers, whereas, in AI, we can achieve ultimately highly precise classification or prediction, that cannot be possible by existing technologies, by applying machine learning techniques, such as deep learning, against a massive training data. The project office for AI & big data was started in FY2017. The mission covers promoting applications of big data/AI technologies to the research activities in the divisions in the CCS, promoting big data/AI research exploiting supercomputers and promoting collaborations with the center for artificial intelligence research (C-AIR) and other institutes.

The main activities are as follows:

- **Promoting the application of big data/AI technologies to research divisions in computational sciences**

  In various scientific areas, it has become very active to apply big data analysis or machine learning techniques to massive data for discovering new knowledge. One of the most well-known examples is bioinformatics. We promote applications of big data/AI techniques to different research domains in computational sciences by the collaboration between the divisions of computational sciences and the divisions related to big data/AI.

  To this end, we have been periodically organizing talk seminars by inviting speakers from both computer science and scientific domains to promote collaborations (Figure 1).

- **Promoting big data/AI research exploiting supercomputers**

  It is known that substantial computer resources (both CPU and memory) are mandatory to perform big data analysis/AI. For this reason, supercomputers are considered to be one of the most suitable environments for performing big data analysis/AI. Thus, in major supercomputers, the number of such use cases has been growing. We promote to use the supercomputers at CCS in the research activities in big data analysis/AI.

  To this end, we promote utilizing our supercomputers for processing big data/AI workloads. In fact, from this year, Cygnus has been used to process sleep big data. Also, we encourage faculties in the Department of Computer Science to use Cygnus for Deep-Neural Networks (DNNs).

- **Collaboration with the center for artificial intelligence research (C-AIR) and other institutes**

  We promote the collaborations with the center for artificial intelligence research (C-AIR) at our university and other institutes concerning the above activities related to big data/AI.

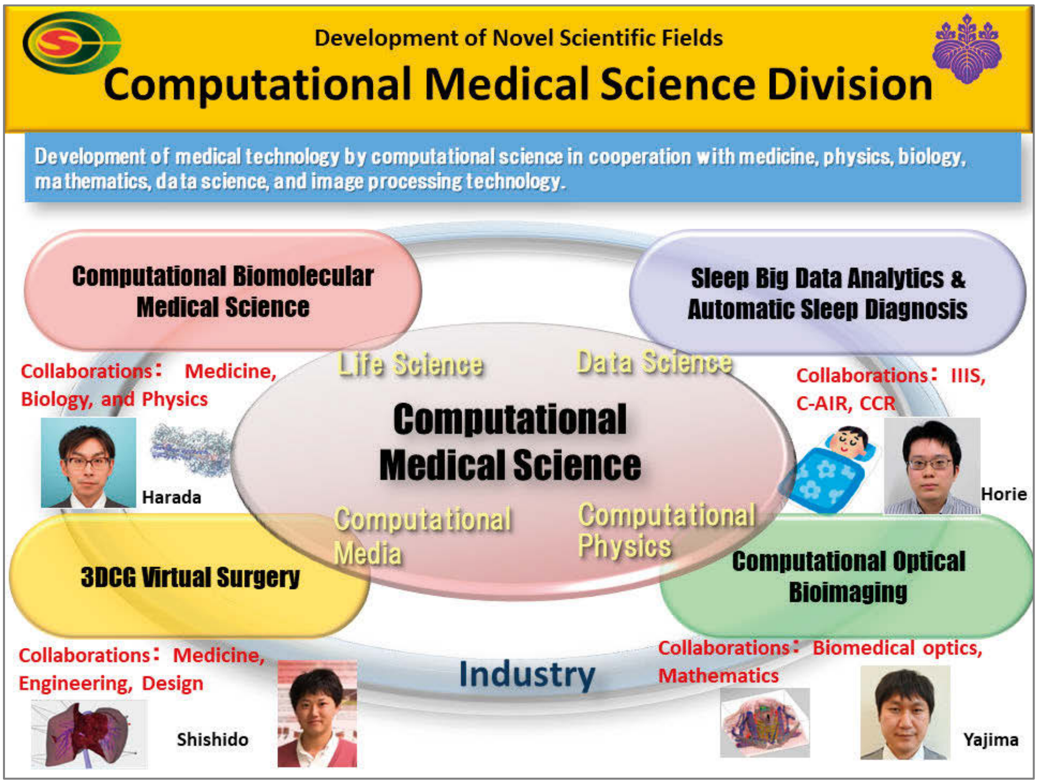
  In 2019, we invited Dr. Tanimura at the Artificial Intelligence Research Center (AIRC), National Institute of Advanced Industrial Science and Technology (AIST), who is in charge of ABCI (AI Bridging Cloud Infrastructure), the world's first large-scale Open AI Computing Infrastructure, to our talk seminar as the speaker.

In the future, we continue the aforementioned activities to promote big data and AI research at CCS.

Figure 1: Talk seminar.

5.7.5 Department of Computational Medical Science

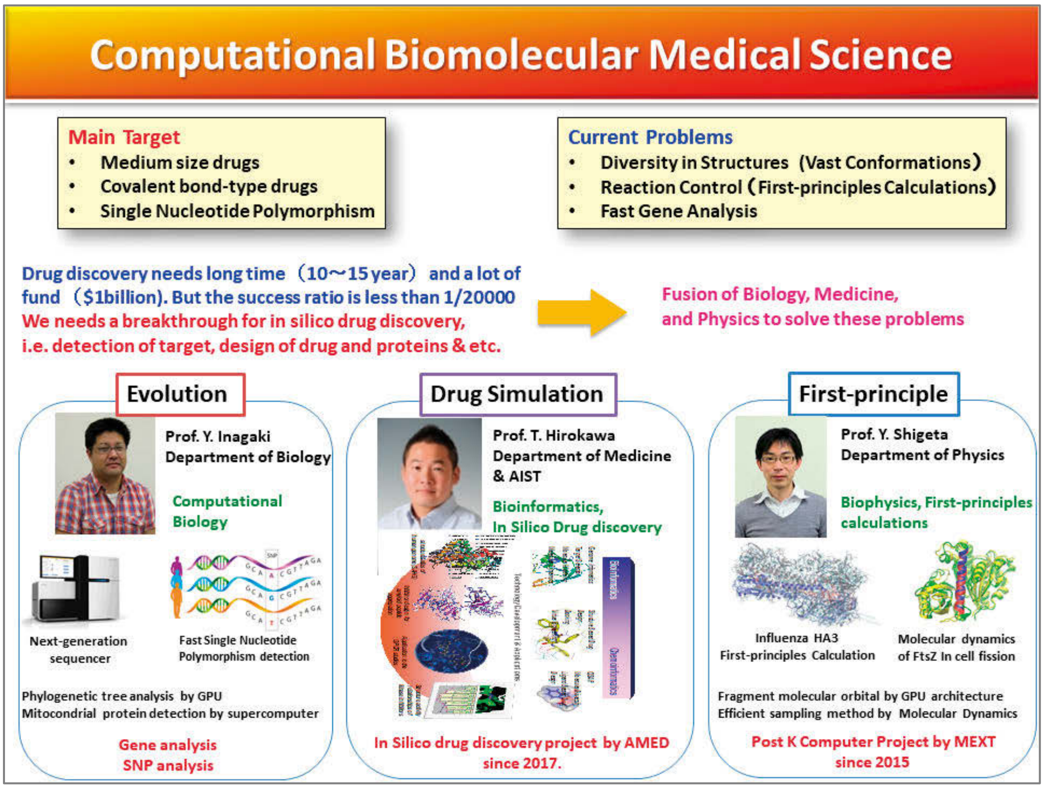
For the development of novel technologies for medical care, there has been hitherto conducted "medicine and engineering cooperation", which is the cooperation between medical scientists in private enterprises and engineers in academic institutes, or medicine, science and engineering cooperation" including natural scientists as well. Owing to recent rapid strides in computational science, state-of-the-art computational techniques have been developed, and they have established an indispensable research method comparable to theory and experiments. Besides, the technology of big data and machine learning has made remarkable progress in the fields of database and computational media. In the Center for Computational Sciences, University of Tsukuba, we promote "**Computational Medical Science**", which initializes a novel approach of "medicine and computation cooperation" by incorporating cutting-edge computational sciences into medical science. In this department, we explore medical technologies based on the latest development of computational methods, imaging technology, and machine/deep learning, in cooperation of computational sciences in physics, life science, database technology, computational media engineering with medical science and industries. For the objectives, we propel four projects of (1) Computational Biomolecular Medical Science, (2) Big Sleep Data Analytics and Automatic Sleep Diagnosis, (3) 3DCG Virtual Surgery, and (4) Computational Optical Bioimaging, in pursuing mutual cooperation and synergy.



1) Computational Biomolecular Medical Science

(by Division of Life Sciences)

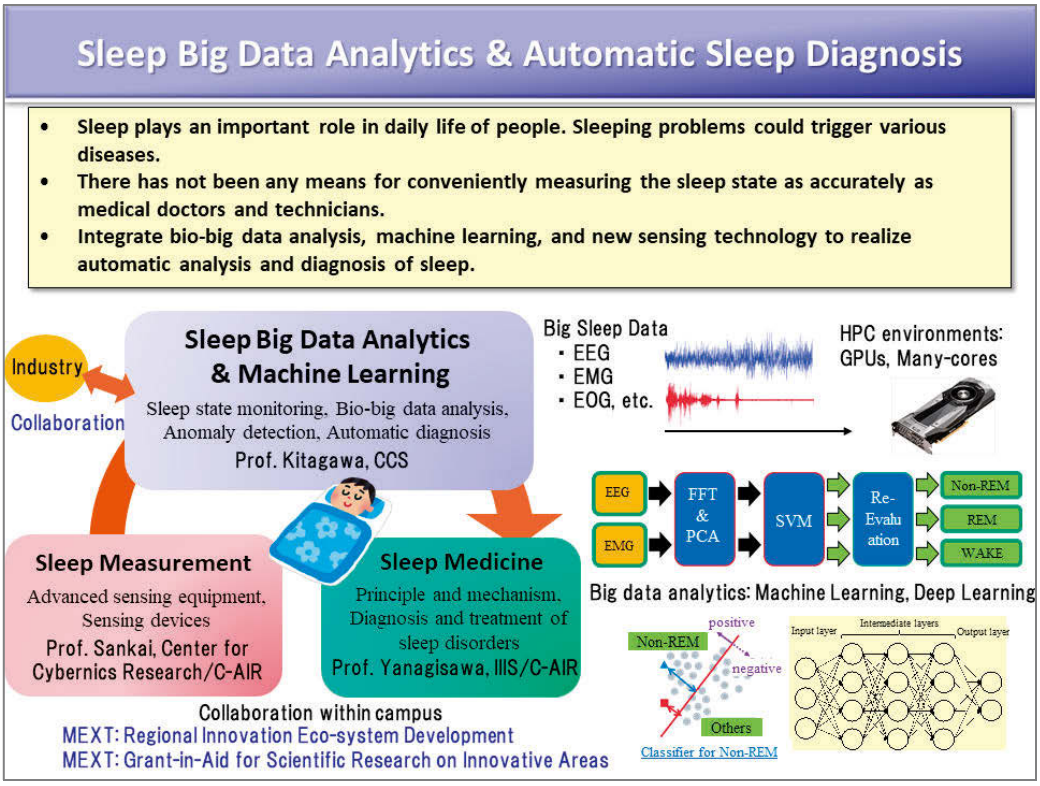
In conventional drug development, one has aimed to develop small molecular drugs with low side effects that have both high selectivity and the binding ability for a specific target. In order to support them, in silico technology has been advanced in recent years, with the expectation that it will be possible to reduce the cost to 100 billion yen per drug for ten years. However, despite many attempts, few cases have been put to practical use because of the limitation of the small-sized drugs. One of the new drug targets is the middle-sized drugs such as cyclic polypeptides and DNA/RNA aptamers. In this group, we conduct research on reaction pathway analysis using first-principles calculation and analysis of substrate-protein binding process using molecular dynamics calculation for drug discovery targeting on middle-sized molecules. In particular, the computational methodologies for the membrane permeability, p*K*a, and redox potential prediction are developed.



2) Big Sleep Data Analytics and Automatic Sleep Diagnosis

(by Division of Computational Informatics - Database Group)

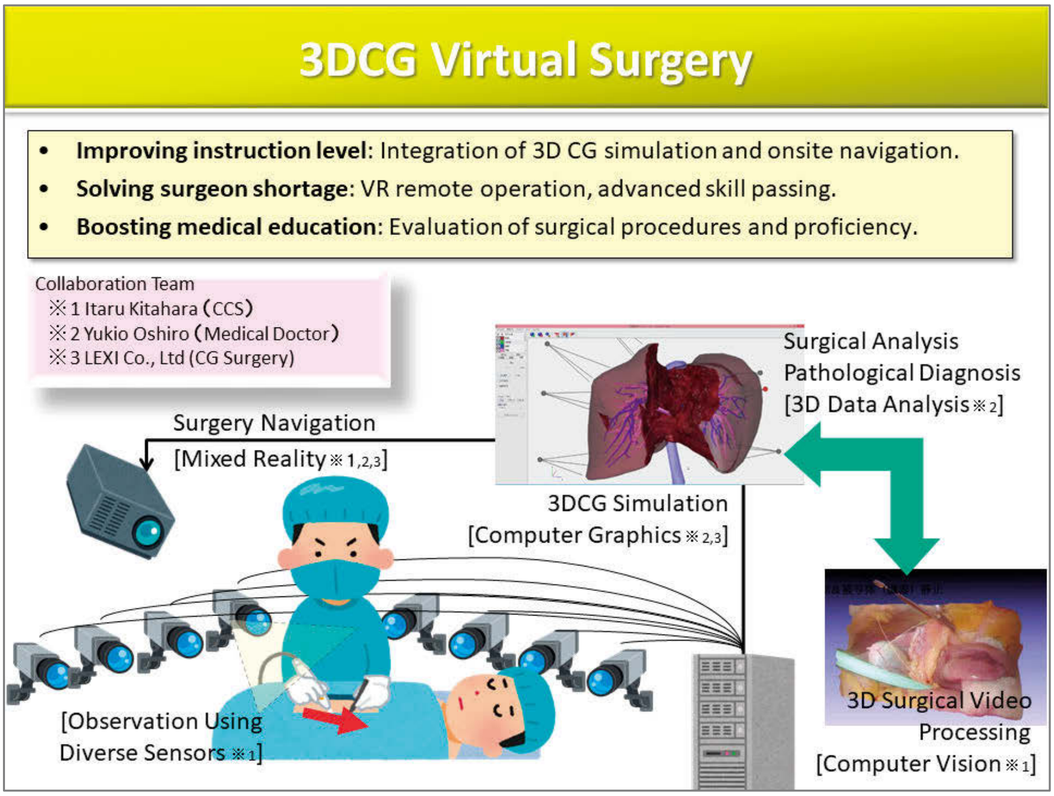
Sleep plays an important role in people's daily lives. Sleep disorders could cause various illnesses. There are a lot of scientific questions that need to be answered about sleep. Quantitative and accurate measurements and analysis of sleep are fundamental issues in sleep research. Sleep polysomnography (PSG) is a commonly used sleep measurement method. PSG attaches many sensors to the subject and continuously measures and records various biological data such as brain waves, respiratory movements, and eye movements throughout the night. In PSG, the burden and cost of the subject are large, and measurement over a long period is impossible. Moreover, analysis of the acquired data depends on manual inspection by human experts, and it is impossible to analyze large-scale data. In response to the increasing social interest in sleep in recent years, some methods have been developed to easily measure sleep status using a smartphone or the like. However, at present, there is still no means to conveniently measure sleep as accurately as human experts. This research aims to realize automatic sleep analysis and diagnosis by integrating sleep big data analysis, machine learning and new sensing technology, and to pioneer a new computational medical science field.



3) 3DCG Virtual Surgery

(by Division of Computational Informatics - Computational Media Group)

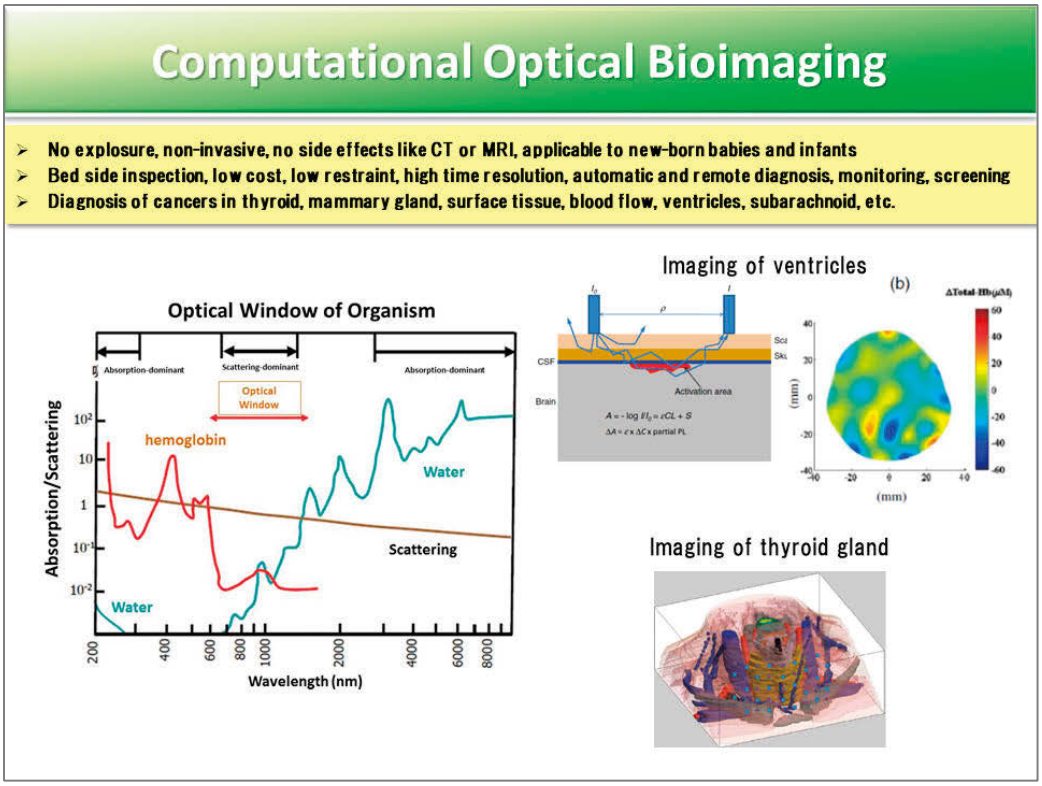
Although the safety of surgery has improved urgently due to advances in medical technology, the upper limit of patient survival is always surgical cancer, the number one cause of death in Japan, and the 1st treatment option is surgery. On the other hand, doctors vary in skills because of increased knowledge and skills that need to be acquired and lost due to medical progress (regional disparities in 5-year survival rates for cancer resection are more than 10%). Since education takes about 15 years, there is a shortage of surgeons and there are concerns that the problem will become even more serious. Until now, research and development on virtual surgery using IT technology have been carried out, however, there are not many implementation examples of surgical navigation systems based on 3D visual information. Our research aims to realize "3D surgical navigation system" that integrates "3DCG simulation" used by doctors for preoperative examination and "on-site navigation" based on 3D Computer Vision technology. Supporting surgeons with an intuitive understanding of proper instructional procedures and advanced medical techniques can improve the level of surgery. In addition, by utilizing technologies such as 3DCG modeling and Augmented Reality (AR), we realize a remote diagnosis and VR treatment system, which aim to correct regional disparities in medical technology. Furthermore, by applying our technologies to laparoscopic surgery, a surgical procedure with a less physical burden on the patient can be possible.



4) Computational Optical Bioimaging

(by Division of Astrophysics)

In recent years, the technology of optical imaging is extraordinarily developing, and thereby molecular processes in live cells and tissues can be pursued. At present, the imaging methods such as X-ray CT or MRI are widely applied, and mainly detect the alteration of morphology at a level of organs and tissues. However, these methods are subject to the risk of significant exposure and require a large-scale apparatus or a specialized measurement room. On the other hand, the optical imaging can dynamically visualize multi-level function and morphological alteration in molecules and organs, and possesses a lot of advantages such as no exposure, non-invasion, bed side inspection, low cost, low restraint, and high time resolution. Thus, it allows us to make automatic and remote diagnosis, monitoring, and screening and is applicable to new-born babies and infants without side effects like CT or MRI. Since biological tissues are strong scattering media, a sophisticated technology of computational science is required to extract the local information from scattered light. The study for practical realization in clinical settings has not been thitherto sufficient. In this project, we aim at developing a safe technology of CT with near-infrared imaging under the cooperation among the construction of light propagation models based on the radiative transfer equation (RTE), the inverse-problem analysis based on mathematical methodology, and the experiments of medical optics for biological tissues.



5.7.6 Liaison Office for Multidisciplinary Computational Sciences

The Center for Computational Sciences (CCS) conducts research activities grounded in the central concept of “Multidisciplinary Computational Science” through collaboration and cooperation among various computer-related and scientific fields. The Liaison Office for Multidisciplinary Computational Sciences is a key part of the Center’s efforts aimed at maintaining its position as an international hub for computational science information.

■ Cooperation among Different Fields

In order to promote multidisciplinary computational science, cooperation among different fields is essential. In 2011, using the research results of first-principles electronic state calculation for 100,000 atom silicon nanowires using K computer, a research group from RIKEN, University of Tsukuba, the University of Tokyo, and Fujitsu Limited won the Gordon Bell Prize for Peak-Performance, which is recognized as an outstanding achievement in high-performance computing. This is just one of the results of cooperation among different fields that have taken place at the Center for the past years.

■ International Cooperation

As for international cooperation, partnership agreements have been concluded between University of Tsukuba and the University of Edinburgh in the UK, as well as with Lawrence Berkeley National Laboratory in the US. Furthermore, as part of the efforts to deepen the computational science research exchanges, the CCS and the University of Edinburgh Parallel Computing Centre (EPCC) are currently hosting joint symposiums, and the Center is cosponsoring workshops with Lawrence Berkeley National Laboratory.

■ Multidisciplinary Pioneering Program

The multidisciplinary pioneering program encourages the promotion of research efforts that require collaboration and cooperation among divergent scientific fields. Cooperation between the computational physics (science) and numerical analysis (engineering) fields in order to implement calculation code with high execution efficiency and to perform the necessary large-scale simulations using the code is one of our program activities. There are also projects that aim at new research deployments and developments by facilitating organic cooperation among different fields utilizing the same techniques in computational science. The multidisciplinary pioneering program has support from the collaborative multidisciplinary program of the Center.

■ Organization for Collaborative Research on Computational Astrobiology

In the last decade, the field of "Astrobiology" has attracted a significant deal of attention owing to advanced observations of extrasolar planets as well as interstellar molecules. This organization aims at the creation of a *computational astrobiology* by exploring key processes related to the origin of life in the universe through *ab initio* calculations based on collaboration among the Computational Astrophysics, Computational Biology, Computational Planetary Science, and Computer Science fields. These research efforts are focusing on the analysis of the potentials of interstellar molecular biology, planetary biology, and the astrophysics of star and planet formation.

5.7.7 Promotion Office for Computational Sciences

The Promotion Office for Computational Sciences promotes the personnel development program associated with computational sciences in collaboration with the graduate schools, and contributes to society by disseminating information concerning the advanced research conducted at this Center.

■ Personnel Development

・Graduate School Dual Degree Program

The graduate school consists of master's programs and doctoral programs. Doctoral candidates usually study a specialized field through both programs. However, since sophisticated computer skills and experience are necessary for advanced research in scientific fields such as physics, global environment, and biology, a broad level of expertise in both science and computer technology is required for computational science doctoral candidates.

The Promotion Office for Computational Sciences promotes dual degree programs to meet this need. The dual degree program makes it possible to obtain a doctorate in a scientific field along with a master's degree of computer science simultaneously, by a doctoral program in scientific field and a master's program in computer science.

・Computational Science English Program

In response to the increasing numbers of international students from overseas, the Computational Science English Program was established as a master's program in computer science that can be completed in English. As shown in the table, this program provides English lectures in 13 subjects, along with English language research guidance aimed at assisting master degree candidates in successfully obtaining their degrees.

・Campus-wide Courses for Graduate Students

Since computer technology is the foundation of all research activities in graduate schools, classes in computational science literacy and high-performance parallel computing technology for computational science have been established as common subjects for all graduate students. These are open to outside researchers and students from other universities.

■ Social Contribution

・Cooperation with other institutions

Domestically, research cooperation in the field of high performance computational technology is advanced under the T2K Alliance that connects University of Tsukuba with the University of

Tokyo and Kyoto University, along with the close research cooperation ties with other research organizations within Tsukuba City. We have also built an international research cooperation framework through the International Lattice Data Grid (ILDG), which is an international data-sharing project of particle physics, with the University of Edinburgh (UK), Lawrence Berkeley National Laboratory (US), and others. We intend to further strengthen and develop the domestic and international research cooperation, and to utilize those relations as a bridge among researchers and exchange students to pursue collaborative research.

・Mt. Tsukuba Project

This project supports research and educational activities, while contributing to society, by continuously observing, recording, and disseminating weather observations (temperature and humidity) from the 877 m summit of Mt. Tsukuba.

・Dissemination of Information

Our office produces three types of brochures. One aimed at high school students and above, another aimed at graduate students and above, and the third written in English to meet the needs of our diverse applicants and students. The office also coordinates visits from high school students within Japan and overseas university students, as well as “open house” events that are open to the public. Through these efforts, we work to deepen exchanges with people around Tsukuba City and in the Kanto region. In addition, the faculty members actively offer and promote off-campus classes and lectures.

5.7.8 Bureau of Public Relations and Strategy

Overview

In 2010, the Bureau of Public Relations was established aimed at improving relations with society in order to advance the mission of the Center for Computational Sciences (CCS) and to promote the computational sciences themselves. To that end, three public relations concepts based on the establishment significance of the CCS have been set forth for use in guiding daily operations.

In 2016, The Bureau of Public Relations reorganized to the Bureau of Public Relations and Strategy to aim at succeeding to the concepts, and supporting and promoting strategic projects in the CCS. The Bureau of Public Relations and Strategy cooperates and works with the Promotion Office for Computational Sciences and the Liaison Office for Multidisciplinary Computational Sciences on the support of the research projects and public relations.

Public Relations Concepts

- We will conduct interactive public relations to foster enhanced relationships between the CCS and society.
- We will aim at increasing the reputation of the CCS and the computational sciences.
- We will enhance the level of understanding of the fundamental policies of the CCS, and work to improve the reliability of the CCS.

Activity Results

1) Public Relations

- **Website:** https://www.ccs.tsukuba.ac.jp/
  We renewed our website in 2017 for that a visitor to more easily access the latest information. The website of CCS provides up to date information on researchers, projects, supercomputers, database disclosures, symposiums/seminars and job openings, etc. The website is managed in both Japanese and English and has approximately 10,000 page views per month.
- **Brochures**
  We prepare three types of brochures based on the intended readership: “Computational Sciences and Supercomputer” for the general readers, especially high school students; a Japanese text for professionals above a graduate student; and an English text for professionals. Annual circulation of each brochure was 2,450; 400 and 630 on the average.
- **Tour and Open House**
  Every year, we hold an open house day in April. In addition to this, the CCS accepts campus

tour visitors at any time, which are high school students mainly. In late years, the number of visitors from the overseas increase. The number of visitors was 1,968 in fiscal year 2014; 2,294 in fiscal year 2015; 1,766 in fiscal year 2016; 1,553 in fiscal year 2017; 2,505 in fiscal year 2018; and 2,735 in fiscal year 2019. The visitors from overseas were approximately 130 per year. From 2017, the Bureau of Public Relations and Strategy supports the open house of the Information Technology Center of the University of Tokyo, as a staff of a tour to visit Oakforest-PACS.

- **Media Promotions**

  The number of press releases was 8 in the fiscal year 2014; 0 in the fiscal year 2015; 9 in the fiscal year 2016; 3 in the fiscal year 2017; 6 in the fiscal year 2018; and 5 in the fiscal year 2019. Eleven were also released in English. Many articles based on our releases appeared in a newspaper and an online journal.

- **SNS Promotions**

  Twitter: The CCS opened Twitter account (@CCS_PR) in 2010 for providing the information about symposium/seminar, press release, job opening, and related information concerning the Computer/Computational Sciences, University of Tsukuba and Tsukuba city, etc. The account has gathered 1,933 followers (as of January 2020).

  YouTube: The CCS also opened a YouTube channel in January 2017. The channel has 14 movies (five are in English) and has gathered 4,663 views and 35 followers.

- **InPACS: Interacting Plot of Atomic nuclei & Computed Shapes**

  We supported establishing the website “InPACS: Interacting Plot of Atomic nuclei & Computed Shapes” (http://wwwnucl.ph.tsukuba.ac.jp/InPACS/) in both Japanese and English for the public in response to questions called “What is the nuclear chart?” and “What are the shapes of atomic nuclear?”. We also provide a detailed data set of each atomic nuclear for researchers on that website.

- **Entrance Lobby**

  The Bureau maintains the mini gallery at the entrance lobby. The rack of HA-PACS, the calculation node of Oakforest-PACS, and several descriptions are written in both Japanese and English were added in late years.

2) Project Supports

- **Exhibition booth in SC and ISC**

  The CCS exhibits every year in the exhibition of SC, which is the big conference held in the United States in November. The Bureau manages the booth planning and prepares posters and novelty items. We also support to attend the exhibition of ISC held in Germany in June as a member of JCAHPC.

- **Computational Medical Science**

  At the time of the foundation of the Computational Medical Science Project, we coordinated the CCS and the Faculty of Medicine, University of Tsukuba, to hold the joint symposiums. We will continue to support the project.

- **Mt. Tsukuba Project**

  The Mt. Tsukuba Project, which mainly conducted by the Division of Global Environmental Science, supports research and educational activities, while contributing to society, by continuously observing, recording, and disseminating weather observations at the 877m summit of Mt. Tsukuba. In 2016, the project was placed as a joint project with Tsukuba-san Shrine and University of Tsukuba, and they established the "Meteorological Station of the Tsukuba-san Shrine & Center for Computational Sciences, University of Tsukuba". The Bureau supports the data opening on our website.

Future Plan

The Bureau continues the activities of public relations based on the concepts and support to the many projects proceeded by the all division. We will also support projects drawn up newly by the Strategic Planning Headquarters and will act for the smooth accomplishment of the research and the public relations in the future.

5.8 COMA Project

Motivation and Objective

After we launched the HA-PACS Project at the CCS, we also started another possibility of accelerated supercomputing beside of GPU. Around 2012, Intel started the research on many-core architecture and contracted with institutes in the world on many-core architecture accelerated computing. The CCS contracted with Intel to introduce a computation node with Knights Ferry (KNF) which was a prototype of later commercial many-core acceleration device lead to Intel Xeon Phi series. KNF was provided as an accelerator for ordinary Xeon CPU through PCIe bus. The purpose of KNF was mainly to develop system software stack to be ready for practical accelerator and the performance result was not expected.

After the research level introduction of many-core processor, Intel started to provide a commercial version which was coded as Knights Corner (KNC). The CCS targeted KNC as one of possible accelerator solution after our experience of KNF evaluation. HA-PACS System introduced GPU and FPGA combination was one of the best accelerated computing system because the GPGPU technology was widely applied to many of memory bandwidth bound and regular floating point calculation base applications which occupy one of the most popular category of HPC solutions. However, we considered that still most of users want to program in ordinary manner where OpenMP+MPI was the general programming style rather than CUDA or OpenCL for GPUs. Thus, the CCS launched a new project to introduced many-core base acclerators. For this research plan, MEXT approved to construct a system with US$1.4M. That amount was not enough to aim PFLOPS-class system for practical use of many-core cluster. Finally, University of Tsukuba allowed us to make a product level system helped by MEXT budget.

On the other hand, we launched JCAHPC in 2013 toward the new generation system in Japan which overcomes the performance of K Computer. In the main stream of concept of the machine, we also focused on many-core architecture (see 5.2). However, the goal to introduce such a many-core processor at JCAHPC was to build a "stand alone" many-core system which does not depend on the host CPU but he many-core processor stands as self-bootable main CPU. The processor was finally available as Intel Knights Landing (KNL) and bootable Intel Xeon Phi CPU. Therefore, we introduced a new machine with attached PCIe card version of Intel Xeon Phi (KNC) to make a large scale experimental system for many-core architecture research. The system was named COMA as 9th system in PACS/PAX series (PACs-IX). The name of COMA came from "Cluster Of Many-core Architecture" and also represents a constellation with the same name which is well known as a cluster of galaxies. When we think a single core as a star, a many-core processor seems like a galaxy, and a cluster with many-core processor corresponds to that constellation.

System Overview

In the COMA System, we introduced two cards of KNC (Intel Xeon Phi 7110P) to be connected to the host CPU vie PCIe bus. To enhance the performance of single node, we installed two KNC cards on each node where two sockets of Intel Xeon CPU are installed. The number of nodes is 398 to reach to the total peak performance of 1 PFLOPS.

Figures 1 shows the overview of COMA System, and Figure 2 shows the node block diagram (left) and the top view of computation node (right).

Figure1　Overview of COMA System

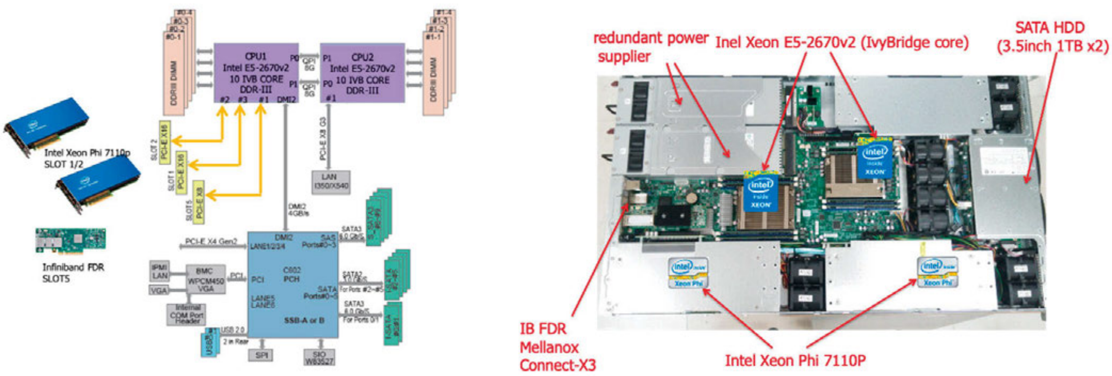


Figure 2　Block diagram of single node (left) and top view photo of single node (right)

Table 1 shows the specification of single node of COMA, and Table 2 shows the system. Here, we introduced InfiniBand FDR to bind all computation nodes as well as Lustre file system to be shared by all computation nodes. The system was installed by Cray Japan.

Table 1 Node specification of COMA

Item	Specification
Computation node	Cray CS300 Cluster Unit with two Xeon Phi
CPU	Intel E5-2670v2 (Ivy Bridge EP)
# of cores	10 cores/socket x 2 sockets = 20 cores/node
Clock	2.5 GHz
Peak performance	400 GFLOPS/node
PCI-express	generation 3 x 80 lanes (40 lanes/CPU)
Memory	64 GiB, DDR3 1866MHz, 4 channel/socket, 119 GB/s/node
MIC	Intel Xeon Phi 7110P
# of MICs/node	2
Peak performance	2.14 TFLOPS/node (1.07 TF/MIC)
Memory	16 GiB/node (8 GiB/MIC)
Interconnection	Infiniband FDR (Mellanox ConnectX-3)

Table 2 Overall system specification of COMA

Item	Specification
Peak performance	1.001 PFLOPS (MIC: 843.9TF, CPU: 157.2TF)
# of nodes	393
File system	Lustre, 1.5 PB user area (DDN SFA12000)
Infiniband network switch	393 port FDR (Mellanox SX6536)
Total network bandwidth	2.75 TB/s
Language	Fortra90, C, C++
MPI	MVAPICH2, Intel MPI
System Management	Cray Advanced Cluster Engine, SLURM

Operation

The COMA System started the operation on April 2013 and ended on March 2019. The system was dedicated to HPCI general program and MCRP of the CCS. In the first year, we configured the system where each node allows job mixing. When a job uses 16 cores of two Xeon CPU only, another job can utilize rest 4 cores of Xeon CPU and two accelerator cards, Intel 7110P many core processor card, simultaneously. This is because we considered to mixture ordinary cluster users and special groups to use many-core accelerators as their challenge for programming of that architecture. However, we found it caused a problem on the batch scheduler (SLURM) and decided not to introduce job mixture. Instead of that, we fully allowed the most advanced users for performance tuning on the next large scale many-core system under JCAHPC.

Actually, a number of applications were tuned on performance to utilize the full feature of Intel's many-core concept. We believed that our experience to use the accelerator card version of many-core processors (KNC) would be a good practice for the stand-alone version of Xeon Phi, KNL. One of the examples was ARTED (Ab-initio Real Time Electron Dynamism simulator) developed at the CCS in the research group of quantum condensed material physics, and the code was finally merged in a large code set under the name of SALMON. Several other applications were also implemented and tuned toward KNL processor, in these days.

Appendix A. Faculty Members of CCS

Director: Taisuke Boku

Deputy Director: Kazuhiro Yabana

Taisuke Boku, Professor

Research topics:
Large scale parallel processing, high performance interconnection, cluster computing, hybrid parallel processing system

Kazuhiro Yabana, Professor

Research topics:
Nuclear physics, computational sciences on atomic, molecular,and optical sciences

(1) Division of Particle Physics

Chief: Yoshinobu Kuramashi

Faculty members

Yoshinobu Kuramashi, Professor

Research topics:

Theoretical and computational studies on strong interact ions using lattice field theories

Tomoteru Yoshie, Associate Professor

Research topics:

Elementary Particle Physics

Naruhito Ishizuka, Associate Professor

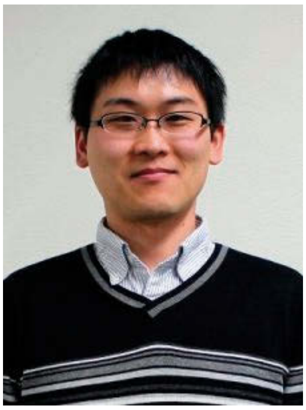
Research topics:

Computational studies on strong interactions using lattice field theories

Yusuke Taniguchi, Lecturer

Research topics:

Lattice gauge theory



Hiroshi Ohno, Assistant Professor

Research topics:

Numerical study on the strong interaction with lattice QCD at finite temperature and density

Sinya Aoki, Visiting Professor

Affiliation:

Yukawa Institute for Theoretical Physics, Kyoto University

Research topics:

Lattice Field Theories, Lattice QCD and its applications to Nuclear Physics

Collaborative fellow

Kazuyuki Kanaya, Professor

Affiliation:

Faculty of Pure and Applied Sciences

Research topics:

Theoretical particle physics, lattice field theory, parallel computers

Takeshi Yamazaki, Associate Professor

Affiliation:

Faculty of Pure and Applied Sciences

Research topics:

Lattice gauge theory

Research staff

- **Naoya Ukita**
- **Yoshimura Yusuke**

(2) Division of Astrophysics

Chief: Masayuki Umemura

Faculty members

Masayuki Umemura, Professor

Research topics:

Theoretical Astrophysics & Computational Medical Science. The formation of galaxies and supermassive black holes, and the optical bioimaging.

Ken Ohsuga, Professor

Research topics:

Theoretical Astrophysics. Black-hole accretion disks and jets, formation of supermassive black holes

Masao Mori, Associate Professor

Research topics:

Theoretical astrophysics, galaxy formation, black-hole accretion flow, astrophysical numerical simulation

Hidenobu Yajima, Associate Professor

Research topics:

Medical physics, Astrophysics, Light propagation in biological tissue, Galaxy formation, Cosmic reionization, Massive black holes

Kohji Yoshikawa, Lecturer

Research topics:

Astrophysics. Theoretical studies on observational cosmology, the formation of galaxies and galaxy clusters, and intergalactic medium

Alexander Wagner, Assistant Professor

Research topics:

Hydrodynamic simulations of AGN feedback in galaxy formation, radio galaxies, and astrophysical jets

Kenji Furuya, Assistant Professor

Research topics:

Astrochemistry

Naohito Nakasato, Visiting Associate Professor

Affiliation:

School of Computer Science and Engineering, Univ. of Aizu

Research topics:

Astrophysical Simulations and High Performance Computing

Research staff

- **Makito Abe**
- **Yuta Asahina**
- **Hajime Fukushima**
- **Shigeki Inoue**
- **Yuichi Takamizu**
- **Satoshi Tanaka**

(3) Division of Nuclear Physics

Chief: Takashi Nakatsukasa

Faculty members

Takashi Nakatsukasa, Professor

Research topics:

Computational nuclear physics, Collective dynamics in quantum many-body systems

Kazuhiro Yabana, Professor

Research topics:

Nuclear physics, computational sciences on atomic, molecular,and optical sciences

Yukio Hashimoto, Lecturer

Research topics:

Microscopic theory of nuclear collective motions

Nobuo Hinohara, Assistant Professor

Research topics:

Double beta decay, Nuclear structure theory, density functional theory, Large-amplitude collective motion in nuclei

Research staff

- **Wen Kai**
- **Bharat Kumar**

(4) Division of Quantum Conensed Matter Physics

Chief: Kazuhiro Yabana

Faculty members

Kazuhiro Yabana, Professor

Research topics:

Nuclear physics, computational sciences on atomic, molecular,and optical sciences

Hiroyasu Koizumi, Associate Professor

Research topics:

Elucidation of mechanism of high temperature copper oxide superconductor and Realization of quantum computer using it.

Tong Xiao-Min, Associate Professor

Research topics:

Atoms, molecules interaction with intense laser field and time-dependent density functional theory

Nobuya Maeshima, Lecturer

Research topics:

Photoinduced phenomena in strongly correlated electron systems

Shunsuke Sato, Assistant Professor

Research topics:

Light-matter interaction and quantum dynamics of matter

Tomoya Ono, Visiting Professor

Affiliation:

Graduate School of Engineering, Kobe University

Research topics:

Development of large-scale first-principles calculation method and computational materials device design

Collaborative fellow

Ken-ichi Hino, Professor

Affiliation:

Faculty of Pure and Applied Sciences

Research topics:

Photophysics of Condensed Matters

Susumu Okada, Professor

Affiliation:

Faculty of Pure and Applied Sciences

Research topics:

Condensed matter physics

Computational material sciences

Research staff

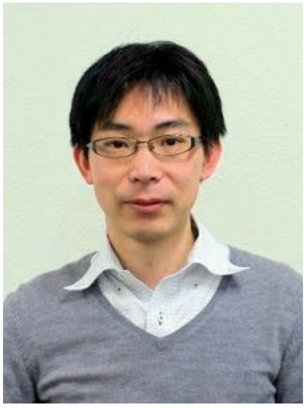
- **Atsushi Yamada**
- **Arqum Hashmi**
- **Yuta Hirokawa**
- **Masashi Noda**
- **Takashi Takeuchi**
- **Shunsuke Yamada**

(5) Division of Life Sciences

Chief: Yasuteru Shigeta

Biological Function and Information Group

Faculty member



Yasuteru Shigeta, Professor

Research topics:

Computational analyses on nano- and bio-systems

Ryuhei Harada, Associate Professor

Research topics:

Life sciences, Biophysics

Mitsuo Shoji, Assistant Professor

Research topics:

Theoretical investigation on the reaction mechanisms of enzymes

Hiroaki Nishizawa, Assistant Professor

Research topics:

QM/MM molecular dynamics for middle molecular drug discovery

Yuta Hori, Assistant Professor

Research topics:

Theoretical studies for proton, electron, and hydride transfer reactions; Theoretical analysis for enzymatic and catalytic reactions; Theoretical studies on organic molecules in interstellar space

Collaborative fellow

Takatsugu Hirokawa, Professor

Affiliation:

Faculty of Medicine

Research topics:

Ryunosuke Yoshino, Assistant Professor

Affiliation:

Faculty of Medicine

Research topics:

Drug discovery and structural optimization using molecular simulation techniques

Research staff

- **Hirotaka Kitoh-Nishioka**
- **Kenji Mishima**
- **Yuki Mitsuta**
- **Kowit Hengphasatporn**

Biological Science Group

Group Leader: Yuji Inagaki

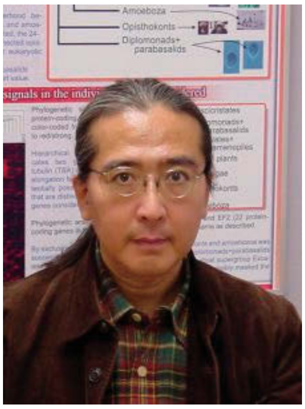
Faculty member

Yuji Inagaki, Professor

Research topics:

Molecular phylogeny of eukaryotes Investigation of lateral genetransfers at the whole-gene and sub-gene levels Estimation of protein functions by combining structural and evolutionary parameters Artifacts in molecular dataanalyses

Collaborative fellow



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CCS Report: PART II

Research Activities of Divisions

2014 – 2019

February 2020

Center for Computational Sciences

University of Tsukuba

Table of Contents

1 Division of Particle Physics

1.1 Overview

Elementary particles have no internal structures. They are not composed of other particles. At present six flavors of quarks, six leptons and Higgs particle are known as the elementary particles in the universe. They interact via four fundamental interactions or forces: gravitation, electromagnetism, the weak interaction and the strong interaction. Among them, the strong interaction, which acts only between the quarks through exchanges of the gluons, shows peculiar features depending on the energy scale. In the high energy region, where the quarks come close to each other, the interaction strength becomes getting weaker (asymptotic freedom) so that the quarks are allowed to move more freely. On the other hand, the quarks are “confined” in the hadrons at the low energy scale. They are never observed individually. Once the energy scale becomes even lower, the protons and the neutrons, which are members of the hadrons, constitute the nuclei in the atoms.

The primary research subject of particle physics group is a large scale simulation of lattice QCD, whose purpose is to investigate its dynamics nonperturbatively based on the first principles. In addition, we have initiated an application of the Tensor Network (TN) scheme to the quantum field theories (QFTs) and some remarkable results are already obtained. In the next subsection we describe the main results for the following research subjects in the past six years:

1) Master field simulation at the physical point in 2+1 flavor QCD,
2) Hadron-hadron interactions,
3) Lattice QCD at finite temperature and density,
4) Application of the TN scheme to QFTs,
5) Numerical study of conformal field theories.

Numerical simulations in the past six years were carried out on T2K-Tsukuba, HA-PACS, COMA, Oakforest-PACS (OFP) and Cygnus in CCS. We also used K computer in RIKEN AICS. At present OFP and Cygnus are in operation. T2K-Tsukuba was a large scale cluster machine, which was installed in June 2008 under the T2K Open Supercomputer Alliance with the University of Tokyo and Kyoto University. This machine was shut down at the end of February

2014. HA-PACS was a large scale GPU cluster consisting of 268+64 nodes, each of which is equipped with two sockets of CPUs and four GPUs. Its operation started in February 2012 and ended in October 2018. COMA was a large scale many-core architecture cluster consisting of 393 nodes, each of which contains two sockets of CPUs and two Intel Xeon Phi (Knights Corner) processors. Its operation started in April 2014 and ended in March 2019. OFP is a massively parallel many-core architecture cluster operated by Joint Center for Advanced High Performance Computing (JCAHPC) which is cooperated by University of Tsukuba and the University of Tokyo. This machine has 8208 compute nodes with the Intel Xeon Phi (Knights Landing) processors and the theoretical peak performance reaches over 25 PFlops. The machine starts operation from December 2016. Cygnus, which is the successor of HA-PACS, is a large scale GPU cluster consisting of 80 nodes. All nodes have two sockets of CPUs and four GPUs and half of them are additionally equipped with two FPGAs. The machine is in operation from April 2019.

Hereafter, [J*] and [P*] referes to the journal papers and the proceedings, respectively, in Sec. 1.5.

1.2 Research Results

1) Master field simulation at the physical point in 2+1 flavor QCD

There are two major problems in lattice QCD simulations. One is that it is still difficult to make a high precision measurement of the physical observables exclusively at the physical point (physical quark masses). They are obtained by extrapolating the results at unphysically heavier quark masses to the physical point, though the results at the physical point are included in some cases. The other is that current lattice QCD simulations determine different physical observables by choosing different sets of gauge configurations. From a view of predictability of lattice QCD it is highly desirable to make a high precision measurement of various physical observables from a unique set of gauge configurations. In order to overcome the above problems, we plan to perform master-field simulations (very large scale simulations at the physical point) so that we can give the reliable predictions for the physical observables relevant for particle physics within and beyond the standard model.

We have initiated the simulation with the Domain-Decomposed Hybrid Monte Carlo (DDHMC) algorithm in 2+1 flavor QCD since the PACS-CS machine started the operation in 2006. We have realized the simulation at the physical point successfully reducing the ud quark mass toward the physical value. After that, we have succeeded in a 1+1+1 flavor QCD+QED simulation on $32^3\times64$ lattice at the lattice spacing of 0.09 fm by incorporating the QED interactions and the up-down quark mass difference with the reweighting method.

The next step was an enlargement of the lattice size in the 2+1 flavor QCD simulation using the K computer. The physical volume is $(8.1\ \mathrm{fm})^4$ near the physical point (m_π=145 MeV), which is much larger than the volume of $(2.9\ \mathrm{fm})^3\times5.8$ fm generated with the PACS-CS machine. The lattice spacing is about 0.09 fm in both cases. We have found a couple of remarkable benefits of large physical volume. Firstly, we observed a clear signal of the $\rho\to\pi\pi$ decay: the effective mass in the ρ channel stays sufficiently below the expected ρ resonance of 770 MeV. Secondly, we have succeeded in reproducing the experimental value of the nucleon charge radius within the error bar using the gauge configurations on the $(8.1\ \mathrm{fm})^4$ lattice. It is known that the precise determination of the nucleon charge radius requires a large spatial volume far beyond $(5\sim6\ \mathrm{fm})^3$. Thirdly, we have found the reduction of the statistical error in proportion to $1/\sqrt{V}$.

In the current project of the PACS Collaboration, we make simulations at the physical point on $(>10\ \mathrm{fm})^4$ lattice with the choice of three lattice spacings to control three major systematic errors in lattice QCD (extrapolation in terms of quark masses, finite volume effect, and finite lattice spacing effect). So far we have finished generating two sets of gauge configurations of (lattice spacing, lattice size)=(0.085 fm, 128^4) and (0.065 fm, 160^4). We are now generating the third set of gauge configurations of (lattice spacing, lattice size)=(0.041fm, 256^4) with a finer lattice spacing. These gauge configurations, which are generated keeping the space-time volumes over $(10\ \mathrm{fm})^4$ in 2+1 flavor QCD at the physical point, are called the "PACS10" configurations. Some physics results with the use of a subset of these gauge configurations are already published. We briefly explain them in the following subsections.

1-1) Finite size effects at the physical point in 2+1 flavor QCD

We have first investigated the finite size effect on the pseudoscalar (PS) meson sector using $(5.4\ \mathrm{fm})^4$ and $(10.9\ \mathrm{fm})^4$ lattices at the lattice spacing of 0.085 fm [J8]. We have tried two kinds of analyses, fixing hopping parameters or measured axial Ward identity (AWI) quark masses. Figures 1 and 2 plot the pion effective mass and the pion decay constant, respectively. Blue symbol denotes the former analysis and red one is for the latter analysis with the aid of the reweighting technique. Comparing the results on two volumes, we have found a sizable finite size effect on the PS meson sector. The former analysis reveals 2.1(8)%, 4.8(1.6)% and 0.36(31)% finite size effect on m_π, m_{ud} and f_π, respectively, on the $(5.4\ \mathrm{fm})^4$ lattice. For the latter analysis, the finite size effect on the PS meson decay constants is 0.66(33)% for f_π, 0.26(13)% for f_K, and 0.40(32)% for f_K/f_π. These values with two-sigma error bars are consistent with the predictions from the full one-loop SU(3) chiral perturbation theory, which are 0.20% for f_π, 0.08% for f_K, and 0.13% for f_K=f_π. The finite size effect on the PS meson masses is hardly detected under the current statistical precision.

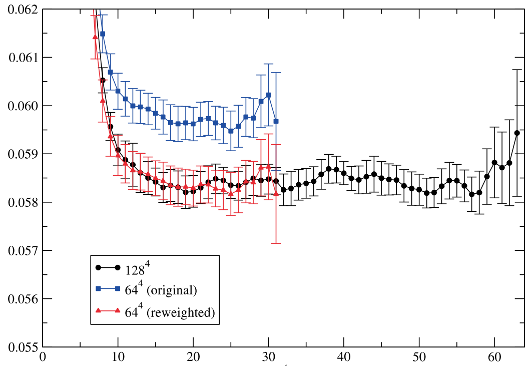

Fig.1. Comparison of pion effective masses on (5.4 fm)^4 and (10.9 fm)^4 lattices.

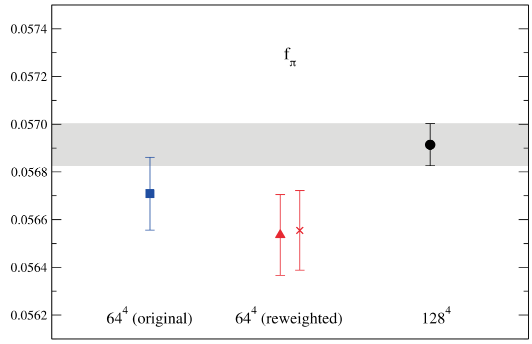

Fig.2. Comparison of pion decay constant on (5.4 fm)^4 and (10.9 fm)^4 lattices.

We have also investigated the finite size effect on the baryon sectors using the same set of gauge configurations as for the PS meson sector [J4]. Comparing the results on (5.4 fm)^4 and (10.9 fm)^4 lattices. The ground states of octet baryons, which are stable on the lattice, show no finite size effect within less than 0.5% level of statistical errors. As an example, we plot the time dependence of the effective masses for the Ξ baryon channel in Fig. 3. For the decuplet baryon sector, we have found no plateau behavior: the effective masses monotonically decrease as the time increases. This is also the case for the Ω baryon channel as depicted in Fig. 4. This is due to a possible mixing with the nearby multihadron states. Since the Ξ baryon mass can be determined with the smallest ambiguity among the baryon masses, we use it together with the pion and kaon masses as the physical inputs to determine the physical point.

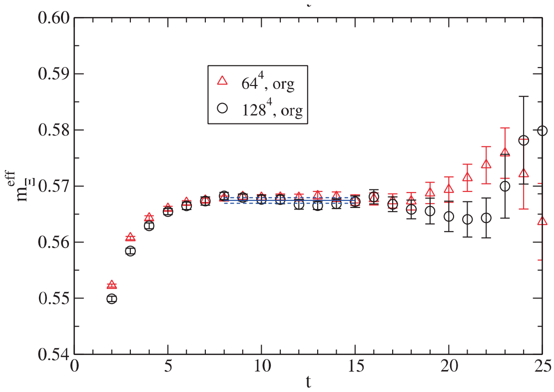

Fig.3. Comparison of effective mass in Ξ baryon channel on (5.4 fm)^4 and (10.9 fm)^4 lattices.

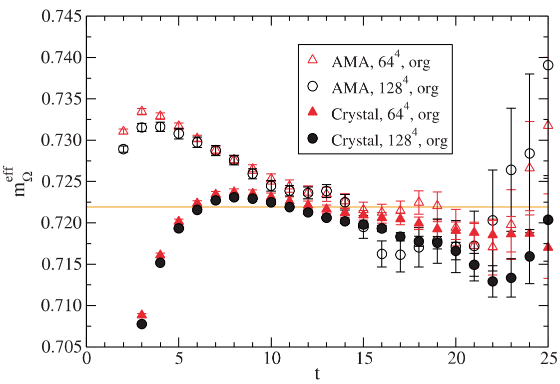

Fig.4. Comparison of effective mass in Ω baryon channel on (5.4 fm)^4 and (10.9 fm)^4 lattices.

1-2) Determination of $|V_{us}|$ from kaon semileptonic decay

One of the urgent tasks of elementary particle physics is the search for signals of physics beyond the standard model. Since the Cabbibo-Kobayashi-Maskawa (CKM) matrix has unitarity in the standard model, the CKM matrix element $|V_{us}|$ is evaluated indirectly using the precisely measured value of $|V_{ud}|$. The value of $|V_{us}|$ is also determined from a semileptonic kaon decay process, K→πlν. However, $|V_{us}|$ cannot be determined only from the experiment. It is required a precise theoretical evaluation of the form factor in this decay process. Lattice QCD can provide reliable values of the form factor from the first principle calculation of the strong interaction. We calculate the form factor at the physical point on a large volume of $(10.9\ \mathrm{fm})^3$ to reduce systematic errors in the lattice QCD calculation. Figure 5 presents our result of the form factors as a function of the momentum transfer squared q^2. Using the value of the form factor at q^2=0 (star symbol in Fig. 5) determined from interpolations of the form factors, we obtain the result of $|V_{us}|$ in this work plotted by the red circle in Fig. 6. Our result agrees with the values of $|V_{us}|$ from the standard model prediction with $|V_{ud}|$ (gray band) and from other kaon decay process denoted by the blue circle and star symbols. The figure also shows that our result is reasonably consistent with recent lattice QCD results from the form factor calculation. In our calculation, the largest systematic error comes from the finite lattice spacing effect. To reduce the systematic error, we plan to repeat the calculation with other subsets of PACS10 configurations at finer lattice spacings.

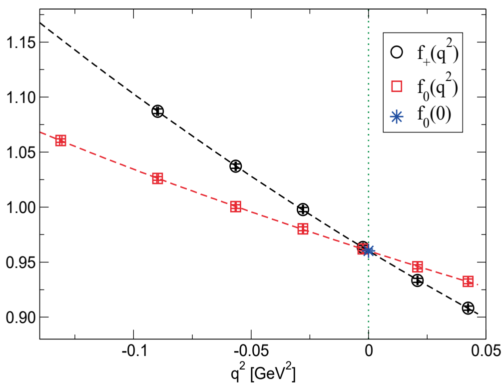

Fig.5. Result for form factors of the semileptonic kaon decay as a function of momentum transfer squared.

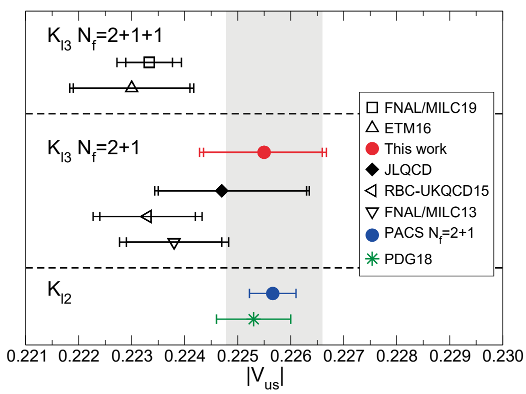

Fig.6. Result of $|V_{us}|$. Red circle expresses our result. Gray band denotes standard model prediction.

1-3) Contribution of hadronic vacuum polarization (HVP) to muon g−2

The muon anomalous magnetic moment $(g-2)_\mu$ has been a key observable to show the predictability of quantum field theory, which the standard model (SM) relies on. The current experimental situation suggests that there might be a sign of the new physics beyond the standard model (BSM) in the muon g−2 anomaly, which is 3 σ to 4 σ deviation between the SM prediction and the BNL experiment in 2004. In order to establish the deviation the new $(g-2)_{\mu}$ experiment is underway in FermiLab aiming at a factor of 4 to 5 improvement from the BNL experiments. However, the high precision experiments are not sufficient for the search of the BSM physics, because the magnitude of theoretical uncertainty in the SM prediction has not been comparable to that in the new experiments yet. The biggest uncertainty left in the SM prediction is coming from the hadronic vacuum polarization (HVP) effect. The lattice QCD calculation is expected to be a promising tool to evaluate the HVP effect based on the first principle. Since the high precision prediction is required for the lattice QCD calculation, we have investigated three major systematic uncertainties using a subset of PACS10 configurations: the finite volume (FV) effect, the cutoff effect and integration scheme dependence [J7]. Our result for the HVP contribution to the muon g−2 is given by $737(9)(^{+13}{}_{-18})\times 10^{-10}$ in the continuum limit, where the first error is statistical and the second one is systematic. Figure 7 is a summary plot of the recent lattice QCD results for the HVP contribution to the muon g−2 in the u, d quark sector. The full quark (u, d, s in 2+1 flavor QCD and u, d, s, c in 2+1+1 flavor QCD) sector is also plotted in Fig. 8. Our result seems to favor the “experimental” HVP value, which is obtained from the BNL experimental value.

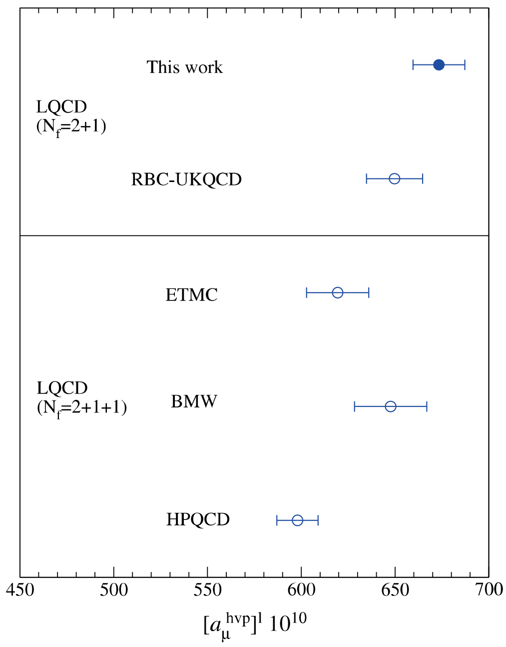

Fig.7. Recent lattice QCD results for the HVP contribution in the u, d quark sector.

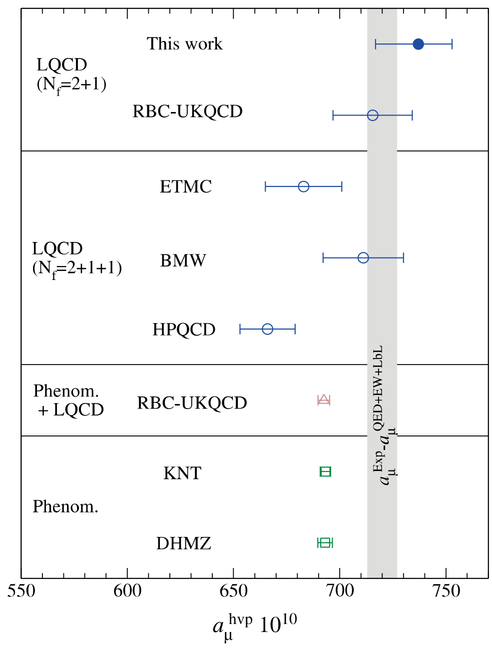

Fig.8. Recent theoretical results for the HVP contribution in the full quark sector. Gray band represents the “experimental” value of the HVP contribution.

1-4) Nucleon electric form factor

The charge radius of proton is measured from two types of experiments: the electron-proton scattering and the Lamb shift of the muonic hydrogen. However, the two types of experiments reported significantly different results by more than five standard deviations, which is called the proton size puzzle. Lattice QCD can provide the value of the charge radius from the first principle calculation of the strong interaction, and give the prediction from the standard model. For this purpose, we calculate the nucleon electric form factor at the physical point on $(10.9\ \mathrm{fm})^3$ [J9]. This large volume calculation allows us to access the form factor in a small momentum transfer region. It is a great advantage of the charge radius calculation because the radius is obtained from the derivative of the form factor at the zero momentum transfer. Our result of the isovector nucleon form factor (square and circle) is presented in Fig. 9 together with the fit result. The figure shows that we improve the statistical error of the form factor compared to our previous calculation denoted by the diamond using several calculation techniques, such as the all-mode-averaging (AMA) method. The isovector charge radius is obtained using several fit forms of the form factor, whose results are summarized in Fig. 10. Our results are roughly 10% smaller than the two experimental results. We will continue the calculation of the form factor to reduce both statistical and systematic errors using the PACS10 configurations.

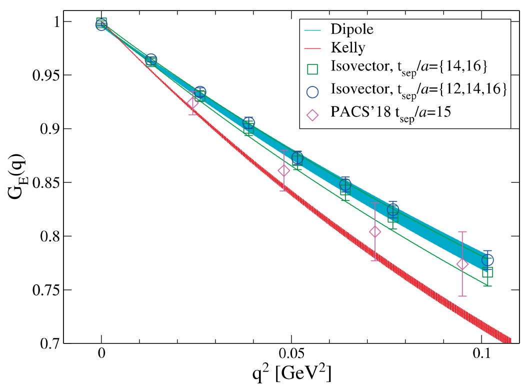

Fig.9. Isovector nucleon electric form factor as a function of the momentum transfer squared.

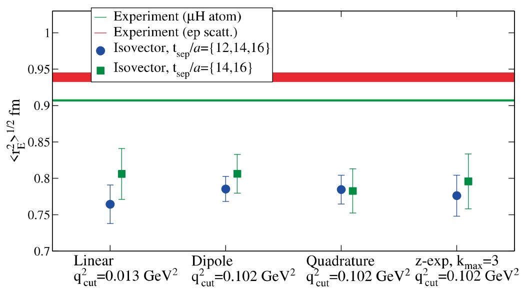

Fig.10. Isovector charge radius determined with four fit forms compared with the experiments.

2) Hadron-hadron interactions

2-1) Direct construction of nuclei from quarks

The strong interaction dynamically generates a hierarchical structure: three quarks are bound to form a nucleon with an energy of 1 GeV, and nucleons are bound to form atomic nuclei with a binding energy of about 10 MeV per nucleon. Since all nuclei are ultimately made of quarks and gluons, lattice QCD should help us quantitatively understand the structure and property of known nuclei based on its first principles. This direct approach will be more important and indispensable if we are able to extract reliable predictions for experimentally unknown nuclei in the neutron rich regions of the nuclear chart. In 2010 we carried out a first successful attempt to measure the binding energies of the ^{4}He and ^{3}He nuclei in quenched QCD with a rather heavy quark mass corresponding to 0.8 GeV pion mass. This calculation was followed by N_f=2+1 QCD calculation at the pion masses of 0.5 and 0.3 GeV [J46]. We also calculated the energies in two nucleon channels, the spin triplet $^3S_1$ and singlet $^1S_0$ channels, in the same pion masses. In this calculation, we found larger binding energy than the experiment in the $^3S_1$ channel and a bound state in the $^1S_0$ channel, which is not observed in nature. These discrepancies from the experiment are caused by several systematic uncertainties in the lattice calculation. In order to investigate the error coming from the heavier pion mass than the physical point, we calculate the two-nucleon energy near the physical point on (8.1 fm)^3 volume. Figure 11 presents the result of the effective energy shift in the $^3S_1$ channel, which corresponds to the binding energy of deuteron in the infinite volume. Our result in a large time region agrees with an estimate of the experimental energy shift on this volume expressed by the light blue band, although the statistical error is large. This result is obtained from more than 100 thousand measurements, so that it is quite hard to improve the statistical error further. Instead of continuing the calculation, we plan to develop new techniques to reduce the statistical error significantly at the physical point. We also investigate systematic error coming from excited state contributions in the binding energy with high precision measurement of the energy shift at the heavy pion mass of 0.8 GeV [P22,P33]. Figure 12 presents the comparison of the energy shift in the $^3S_1$ channel obtained from the exponential (circle) and wall (square) source calculations. The two calculations have different time dependencies, because their excited state contributions to the energy shift are different. The two results of the effective energy shift denoted by the horizontal dashed lines reasonably agree with each other in the region, where the ground state dominates in each two-nucleon correlation function. The region for each calculation begins from t_R denoted by the vertical dashed line in the figure. From the consistency of the two results we conclude that the systematic error from the excited state contributions is small in our calculation, because it is well known that the wall source needs much larger t_R compared to other sources due to the larger contribution from excited states.

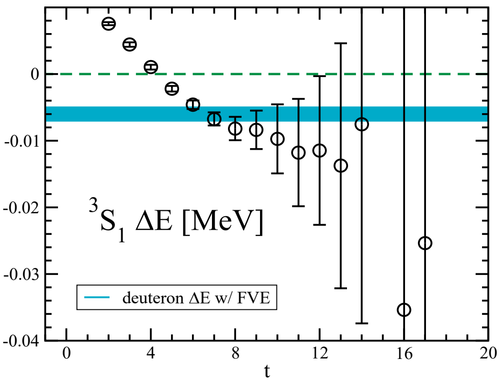

Fig.11. Effective energy shift of the two-nucleon $^3S_1$ channel near the physical point.

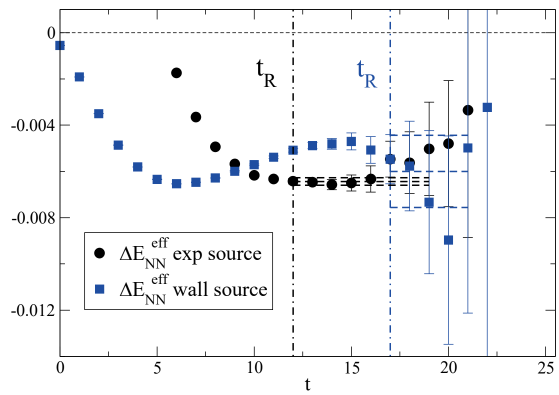

Fig.12. Comparison of effective energy shift between exponential and wall source calculations.

2-2) Two-pion scattering amplitude from Bethe-Salpeter wave function

The scattering phase shift of the two-pion is calculated with the finite volume method in lattice QCD. The method was derived from two-particle wave function in quantum mechanics, and also from the Bethe-Salpeter (BS) wave function. While both derivations are based on the wave functions outside the interaction range *R*, the ones inside *R* is also related to the scattering phase shift through the on-shell scattering amplitude [J27]. We discuss a relation between the BS wave function inside *R* and the half-off-shell scattering amplitude on finite volume [J28]. Furthermore, we calculate the on-shell and half-off-shell scattering amplitudes of the isospin I=2 two-pion scattering system in the quenched lattice QCD at heavier pion masses [J20]. Figure 13 shows that our result of the scattering length from the BS wave function, denoted by H(k;k), completely agrees with the one from the finite volume method, labeled by E_k. We also evaluate the half-off-shell amplitude in Fig. 14. We find that the signal of the amplitude is clear in a wide range of the off-shell momentum.

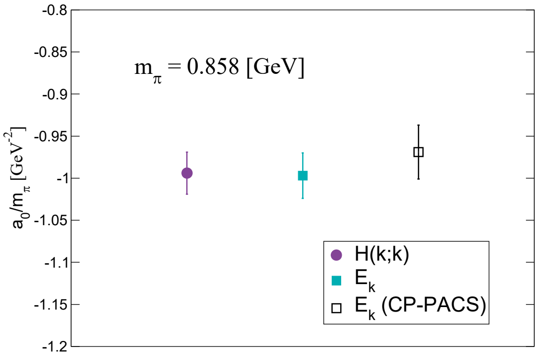

Fig.13. Scattering length from BS wave function (H(k;k)) and finite volume method (E_k).

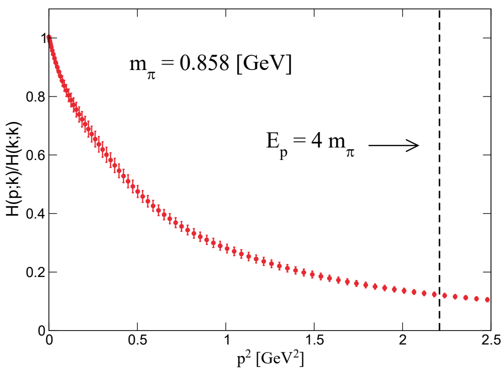

Fig.14. Half-off-shell amplitude from BS wave function as a function of off-shell momentum squared.

2-3) Calculation of $K \to \pi\pi$ decay amplitudes

Calculation of the $K \to \pi\pi$ decay amplitudes is very important to quantitative understand that $\Delta I = 1/2$ rule in the K meson decay and to theoretically predict the direct CP violation parameter ε'/ε from the standard model of the particle physics. A lattice QCD calculation of the decay amplitudes has been unsuccessful for a long time, due to large statistical fluctuations coming from the disconnected diagrams. A first calculation was reported by the RBC-UKQCD collaboration in 2011. Their calculation was carried out with the unphysical kinematics, where the pions in the final state have zero momenta at unphysical quark mass satisfying $m_K = 2\, m_\pi$. In 2015 they reported a calculation with the physical kinematics, where the pions in the final state have finite momenta, at the physical quark mass. They utilized the G-periodic boundary condition in the spacial directions, to extract the decay amplitudes from the $K \to \pi\pi$ time correlation function for the ground state of the two-pion. In all calculations, they used the domain wall fermion action which preserves the chiral symmetry on the lattice.

The Wilson fermion action has been widely used in the lattice QCD calculation. But this fermion action has not been used in the calculations of the K meson decay amplitudes, because it has been considered that unwanted operator mixings occur due to the explicit chiral symmetry breaking and additional calculations are needed to remove the operator mixings. In 2015 we theoretically showed that such operator mixings are absent due to CPS symmetry [J47]. A potential advantage with the Wilson fermion over the domain wall fermion is that the computational cost is smaller. We also reported a first result with the Wilson fermion action in the unphysical kinematics $m_K = 2\, m_\pi$.

In 2018, we extended our calculations to those in the physical kinematics [J21]. In order to extract the decay amplitudes from the time correlation function for the ground state of the two-pion, we consider the process $K(p) \rightarrow \pi(p)\pi(0)$ in the nonzero momentum frame in the periodic boundary condition in the spacial directions. An advantage of our new method over the G-periodic boundary condition adopted by the RBC-UKQCD collaboration is those gauge configurations, generated previously with the periodic boundary condition for the other physics study and published on some databases, can be used. Our final results of the decay amplitudes at $m_\pi = 260\ \mathrm{MeV}$ are

Re A_0 = (51.3 ± 27.5)×10^{-8} GeV , Re A_2 = (2.431 ± 0.019)×10^{-8} GeV

Re(ε'/ε) = (1.94 ± 5.72)×10^{-3} .

We see a large enhancement of the $\Delta I = 1/2$ process and the result of Re$(\varepsilon'/\varepsilon)$ is consistent with the experiment (1.66 ± 0.23)×10^{-3}. But our results still have large statistical errors. Improving statistical error by using a more efficient operator for the I=0 two-pion state for a precise determination of the decay amplitudes is left in the future.

3) Lattice QCD at finite temperature and density

3-1) Determination of critical end point in 3 flavor QCD with Wilson-type quark action

Establishing the QCD phase diagram spanned by the temperature T and the quark chemical potential μ in a quantitative way is an important task of lattice QCD. We have been working on the determination of the critical end point in the parameter space of temperature, chemical potential and quark mass in 3 flavor QCD using the O(a) improved Wilson quark action and the Iwasaki gauge action. Our strategy is to identify at which temperature the kurtosis of physical observable measured at the transition point on several different spatial volumes intersects. This method is based on the property of opposite spatial volume dependences of the kurtosis at the transition point between the first order phase transition side and the crossover one. We have investigated the lattice spacing dependence of the temperature T_E and the pseudoscalar meson mass $m_{PS,E}$ at the critical end point by systematically changing the temporal extent of the lattice with N_T=4,6,8 [J59],10 [J30],12. Figure 15 and 16 shows the continuum extrapolation of $m_{PS,E}$ and T_E, respectively, as a function of $(1/N_T)^2$. We observe a strong cutoff dependence for $m_{PS,E}$ so that we conservatively quote an upper bound $m_{PS,E}/T_E \lesssim 0.93$ in the continuum limit. On the other hand, the continuum limit for the critical temperature is smoothly taken and we obtain T_E=134(3) MeV.

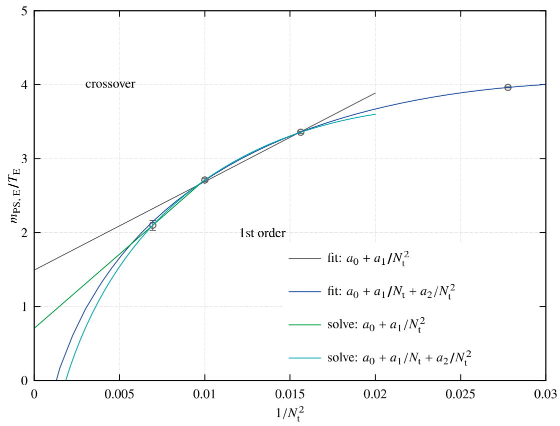

Fig.15. Continuum extrapolation of $m_{PS,E}/T_E$.

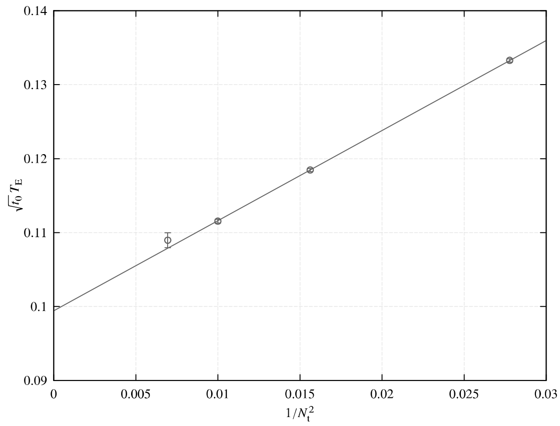

Fig.16. Continuum extrapolation of T_E.

3-2) Study of thermodynamics of QCD applying the SF*t*X method based on the gradient flow

The gradient flow (GF) is a modification of fields according to a flow equation in terms of a fictitious time (flow-time) t. Fields at $t > 0$ can be viewed as smeared fields averaged over a mean physical radius of $\sqrt{8t}$ in four dimensions. Salient features of the GF are the UV-finiteness and the absence of short-distance singularities in the expectation values of operators constructed by flowed fields at $t > 0$. This finiteness enables us to identify these expectation values and corresponding operators as renormalized ones. At small t, these flowed operators can be expanded in terms of operators at $t = 0$ in a conventional renormalization scheme such as the MS-bar scheme. By inverting the relation, we can also expand correctly renormalized physical observables in conventional schemes in terms of flowed operators. Thanks to the asymptotic freedom of QCD at small t, we can calculate the matching coefficients relating to the operators in two schemes by perturbation theory.

The basic idea of the SF*t*X method (small flow-time expansion method) is that, because the flowed operators are finite, we can evaluate their expectation values directly on the lattice without further renormalization. We can thus extract the values of correctly renormalized physical observables by extrapolating proper combinations of expectation values in the GF-scheme to the small flow-time limit $t \to 0$. The method is also applicable to observables whose founding symmetry is violated explicitly on the lattice, provided that the lattice theory has the correct continuum limit in which the symmetry is restored. We are thus applying the method to QCD with dynamical Wilson-type quarks to cope with the problems due to explicit violation of the chiral symmetry on the lattice.

(a) We first applied the SF*t*X method to 2+1 flavor QCD with slightly heavy u, d quarks and approximately physical s quark. In the left panel of Fig. 17, we show the result of the entropy density calculated from the energy-momentum tensor (EMT). The SF*t*X method enables us to calculate EMT in spite of the explicit violation of the Poincare invariance on the lattice. Red circles are the results of the SF*t*X method and black triangles are the results of the conventional integral method to calculate the equation of state. We find that these completely different estimations are well consistent at $T < 280$ MeV. The disagreement at $T > 300$ MeV ($N_t \leq 8$, where N_t is the temporal lattice size) suggests contamination of $O(\,(aT)^2 = 1/N_t^2\,)$ lattice artifact. We also found that the chiral condensates bend sharply and the disconnected chiral susceptibilities peaks at $T \approx 190$ MeV which was suggested as the pseudo-critical temperature from other observables. See the right panel of Fig. 17 for the disconnected chiral susceptibility [J35,P37].

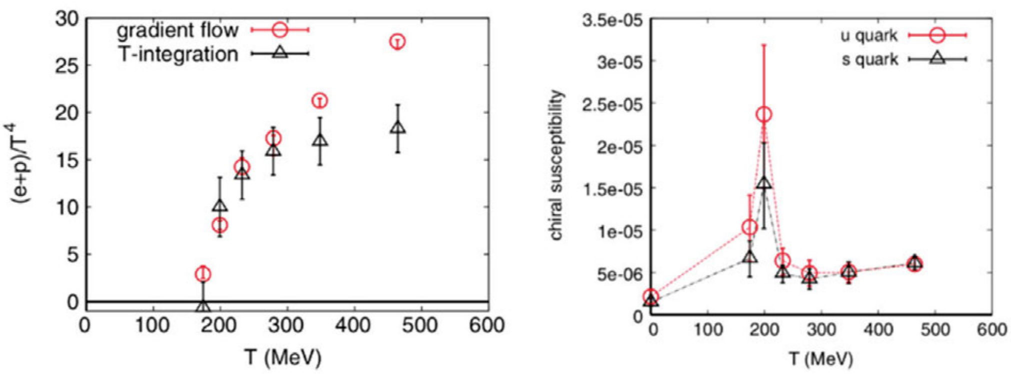

Fig.17. Entropy density (left) and disconnected chiral susceptibility (right) in 2+1 flavor QCD with slightly heavy u, d quarks.

The SF*t*X method also enables us to calculate the topological properties of QCD. Fig. 18 shows our results of the topological susceptibility using gluonic and fermionic definitions. In conventional lattice calculations, the two definitions largely disagree at finite lattice spacing due to the violation of the chiral symmetry. From Fig. 18, we found that the topological susceptibilities estimated with the gluonic and fermionic definitions agree well with each other at $T < 280$ MeV even at finite lattice spacing of $a = 0.07$ fm. These suggest that the SF*t*X method is powerful in calculating observables from lattice simulations [J34,P38].

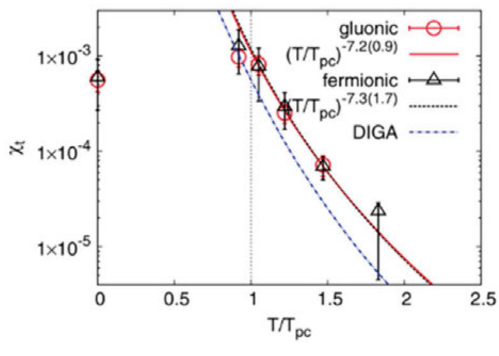

Fig.18. Topological susceptibility in 2+1 flavor QCD with slightly heavy u, d quarks.

(b) We are extending the study to 2+1 flavor QCD with physical u, d, s quarks. Our preliminary results obtained on a slightly coarser lattice of a = 0.09 fm have been presented in Lattice symposia. We found that, with the appropriate choice of the renormalization scale for the matching coefficients, the SF*t*X method works well also on this coarser lattice. Our preliminary results suggest that the transition temperature is around 122-146 MeV at the physical point [P5,P20,P24,P43].

(c) We are also extending the study to other thermodynamic observables, including the viscosities calculated from the correlation function of EMT and the latent heat at the first order transition temperature in QCD with heavy quarks [P4,P6,P15,P16,P17,P21,P25,P36,P66].

3-3) Study of thermodynamics of QCD with Kogut-Susskind quarks

Exploring the phase diagram of QCD at non-zero temperature and density is important to understand properties of strong interaction matter under extreme conditions realized in the early universe, inside of neutron stars as well as ultra-relativistic heavy ion collisions. In collaboration with researchers mainly at Bielefeld University in Germany and Brookhaven National Laboratory (BNL) in the US (so-called HotQCD Collaboration), we have studied the phase structure of QCD with full lattice QCD simulations using the Highly Improved Staggered Quark action. The simulations were done with dynamical quarks having physical strange and around physical light quark masses. Our large data sets with several lattice spacings are able to take the continuum limit as well. At non-zero density, or in other words, non-zero quark chemical potential, standard Monte Carlo techniques cannot be applied due to the so-called sign problem. Our approach to avoid this problem is to calculate observables in terms of a Taylor expansion series around vanishing chemical potential.

In 2014 we calculated strangeness/charm fluctuations and their correlations with net baryon number fluctuations [J57,J58]. Then, we compared the results with predictions from two hadron resonance gas (HRG) models using different strange/charm hadron content and found that an HRG model with the experimentally established strange/charm content cannot describe the lattice QCD results while one with additional strange/charm content predicted by quark model calculations has good agreement with the results at temperatures below the QCD crossover, which suggests presence of these additional states experimentally not observed yet. In 2016 we calculated the mean and variance of net baryon number and net electric charge distributions [J44], which were compared with results from STAR and PHENIX experiments at Relativistic Heavy Ion Collider (RHIC) in BNL. This direct comparison between experimental data and numerical calculations allowed to determine the freeze-out temperature at vanishing baryon chemical potential as well as, for the first time, constrain the curvature of the freeze-out line. We also computed the QCD equation of states at non-zero density using up to the 6th order coefficients of Taylor expansions in the baryon, strangeness and electric charge chemical potentials in 2017 [J33].

The difference between results using up to the 4th and 6th order coefficients showed that truncation errors are small for the baryon chemical potential less than twice the temperature. Using these expansion coefficients, we also estimated the location of the QCD critical point and found that the existence of the critical point is disfavored within our calculations. In the same year we extended our previous calculations on the net baryon number fluctuations to the higher order cumulants including skewness and kurtosis using the next-to-leading order Taylor expansions [J31], where we found that our results are qualitatively similar to the corresponding experimental results for beam energies of $\sqrt{s_{NN}} \geq 19.6$ GeV. In 2019 we showed results on pseudo-critical temperatures of QCD crossovers at zero and non-zero baryon, strangeness, electric charge and isospin chemical potentials [J11], where we obtained a precise value of the pseudo-critical temperature at the zero chemical potential, 156.5±1.5 MeV, and curvature coefficients of pseudo-critical lines in the continuum limit.

4) Application of the TN scheme to QFTs

Since the end of the 1970s, computational particle physics has been led by lattice QCD simulations which were expected to be an ideal tool to understand the nonperturbative dynamics of strong interactions from first principles. Both the algorithmic development and the increase of the performance of the supercomputer over the past 40 years allow us to make simulations with the physical up, down and strange quark masses. We are now able to predict physical quantities associated with single hadrons with high precision. As for hadron-hadron interactions, it is possible to measure the binding energies of light nuclei, which are fundamental quantities in the strong interactions. Although these achievements are remarkable, we all know that the following essential algorithmic problems are left behind:

(a) Sign problem: Current typical lattice QCD simulations are performed with 2+1 flavors of quarks, where the up and down quarks are artificially degenerated keeping the strange quark independent ($m_s \neq m_u = m_d$). This is an algorithmic technique to avoid the sign problem originating from the light u, d quarks. In case that we treat the light quark masses independently ($m_u \neq m_d$), the algorithm employed in current lattice QCD simulations allows negative Boltzmann weight in the path-integral, which makes it difficult to interpret the weight as a probability.

(b) Complex action problem: The lattice QCD studies on the strong CP problem and the finite density QCD demand us to simulate the systems with complex actions. In the former case the so-called θ-term (topological term) added to the conventional QCD action yields a complex number. In the latter case an introduction of non-zero chemical potential μ causes the complex action problem. Although the problem, which is essentially a variant of the sign problem, is inevitable in studying the strong CP problem and the finite density QCD, we still do not have an effective solution to it.

(c) Computational cost to simulate fermionic systems: It is widely known that the lattice QCD simulations require a huge computational cost. This may be less serious compared to the above two problems. But this problem also originates from an essential property of the Monte Carlo approach that the Grassmann numbers cannot be directly treated. After the analytic integration of the fermion fields expressed with the Grassmann numbers, we reconstruct the effective action for lattice QCD using the fictitious boson fields instead of the fermion fields, with which practical simulations are carried out. The effective action, however, results in a non-local form with the fictitious boson fields, whereas local in the original fermion action. This is the reason why the computational cost is demanding in current lattice QCD simulations.

These are essential defects of the Monte Carlo approach in the lattice QCD simulations. In other words, the fundamental solution to these problems cannot be expected as far as we play within the Monte Carlo approach.

The Tensor Network (TN) scheme, which shows evolutional development across various fields after the year 2000, is theoretical or numerical approaches to make a high precision analysis of the many body problems with the tensor network formulation. This scheme has fascinating advantages over the conventional numerical algorithms including the Monte Carlo method: (i) no sign problem and no complex action problem, (ii) logarithmic volume dependence of computational cost (computational cost in proportion to log(V) with V the system size), (iii) direct treatment of Grassmann numbers, (iv) direct measurement of the partition function itself. In the past several years we have been trying to apply the TN scheme to elementary particle physics focusing on the tensor renormalization group (TRG) algorithm, which was originally proposed in the field of condensed matter physics in 2007. We explore the new frontier of research subjects with the TN scheme, such as, the phase structure of the finite density QCD and the strong CP problem, where the conventional Monte Carlo approach was not allowed to access due to the sign problem.

The history of this project essentially started since we developed the Grassmann version of the TRG algorithm (GTRG), which enables us to deal with the Grassmann variables directly, and successfully applied it to the analysis of the phase structure of one-flavor lattice Schwinger model (2D QED) with and without the θ term [J61,J62]. This was the first successful application of the TN scheme to a Euclidean lattice gauge theory including fermions. We explicitly showed that the GTRG algorithm solves all the three problems (a), (b) and (c) explained above by using the Schwinger model as a testing ground. Since then, we have accomplished the following important achievements:

- Discovery of Berezinskii-Kosterlitz-Thouless transition in one-flavor lattice Schwinger model [J23]

- Confirmation of first-order phase transition in two-dimensional U(1) gauge theory with a θ term [J3]
- Confirmation of Silver Blaze phenomenon in two-dimensional complex ϕ^4 theory at finite density [J2]
- Precision measurement of critical coupling in two-dimensional real ϕ^4 theory [J14]
- Construction of TN formulation for two-dimensional lattice N=1 Wess-Zumino model [J24]
- Precision analysis of finite temperature transition for three-dimensional Z_2 gauge theory [J6]
- Discovery of first-order phase transition in four-dimensional Ising model [J5]

In order to show that the TRG method is free from the sign problem, let us present our recent results for the analysis of the two-dimensional complex ϕ^4 theory at finite density [J2]. This model is known to exhibit the Silver Blaze phenomenon, in which bulk observables are independent of the chemical potential below the critical point. An introduction of the chemical potential μ, however, causes the sign problem so that the conventional Monte Carlo method does not work. Figure 19 plots the averaged phase factor in the Boltzmann weight as a function of μ. We find that the averaged phase factor quickly falls off toward zero as the chemical potential and the volume increase. The sign problem becomes severe as the averaged phase factor decreases from one. For example, the Monte Carlo method is useless in the region of μ> 0.05 on a 256^2 lattice. Figure 20 shows that the μ dependence of the number density <n>. The Silver Blaze phenomenon is clearly observed at a large volume of 256^2.

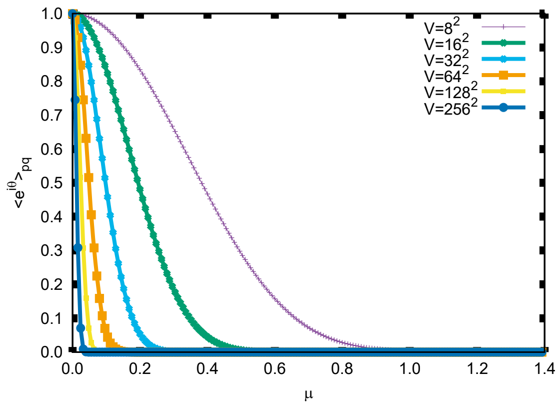

Fig.19. Averaged phase factor as a function of μ. The sign problem becomes severe for larger μ and V.

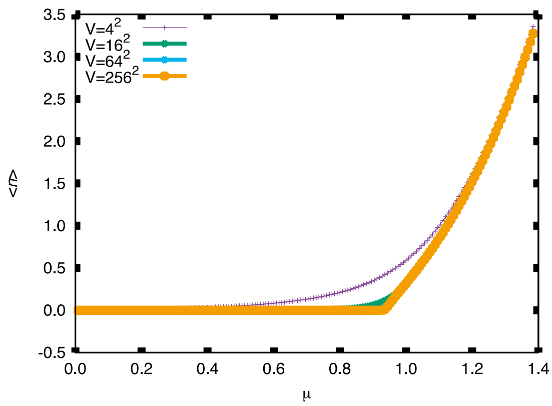

Fig.20. Number density <n> as a function of μ.

5) Numerical study of conformal theories

Conformal symmetry plays a key role in constructing “walking technicolor theories” for

"Beyond Standard Model" of elementary particles. Many flavor QCD (SU(3) gauge theory with N_f degenerate fermions) is expected to have conformal symmetry at zero fermion mass $m_f = 0$ for a certain range of N_f. We have carried out numerical studies of QCD-like theories on a lattice from 2012 to 2017.

In the first stage of our work carried out in 2012 and 2013, we focus on a fundamental issue of "how conformal symmetry looks like on a finite lattice". Numerical study, made on a lattice with finite extent, inevitably introduces a scale which violates conformal (scale) invariance of the theory even at $m_f = 0$. Based on the renormalization group (RG) arguments, we propose a phase structure in $\beta - m_f$ plane ($\beta = 6/g^2$) for "conformal theories with finite IR cutoff" (Λ_{IR}) and confirm it numerically. We find

1. Conformal symmetry at $m_f = 0$ with $\Lambda_{IR} = 0$ extends to finite m_f and forms a "conformal region" with finite Λ_{IR}. The conformal region is separated from usual confining and deconfining phases by a first order phase boundary.
2. Meson propagator in the conformal region takes a form of "power-modified Yukawa-type" $\mathrm{G(t)} \sim e^{-mt}/t^{\alpha}$, instead of exponential form $\mathrm{G(t)} \sim e^{-mt}$.
3. The vacuum of the conformal region is the "Z(3) twisted vacuum", in which spatial Polyakov loops take non-trivial phase.

We have shown for the QCD-like theories that,
<u>there exist conformal regions for $N_f = 7, 8, 12$ and 16, which implies that the conformal window of the QCD-like theory is $N_f = 7 \sim 16$.</u>

In the second stage of our work, starting in 2014, we propose a new method to identify the IR fixed point β^* of QCD-like theories [J54]. From RG arguments, we derive a scaling relation of meson propagators: In terms of effective masses $m(\tau; N) = m_{eff}(\tau, \beta = \beta^*, m_f = 0; N)$, where $\tau = t/N$ is the time separation but scaled by the lattice extent N , the scaling relation leads to $m(\tau; N) = m(\tau; N')$. Namely, scaled effective masses are independent of lattice size at the IR fixed point, while they differ at $\beta \neq \beta^*$. We measure meson effective masses on $8^3 \times 32$, $12^3 \times 48$, $16^3 \times 64$ lattices at various β and find that plots of scaled effective masses overlap to form a universal curve only at a specific β and for $N_f = 7$, 8, 12 and 16. See Fig. 21 for an example. In other words, we have confirmed that,
<u>IR fixed point exists for QCD-like theory within the conformal window N_f =7~16.</u>

Theoretically, we can derive anomalous mass dimension from a scaling relation of propagators themselves, which requires higher statistics than we achieved.

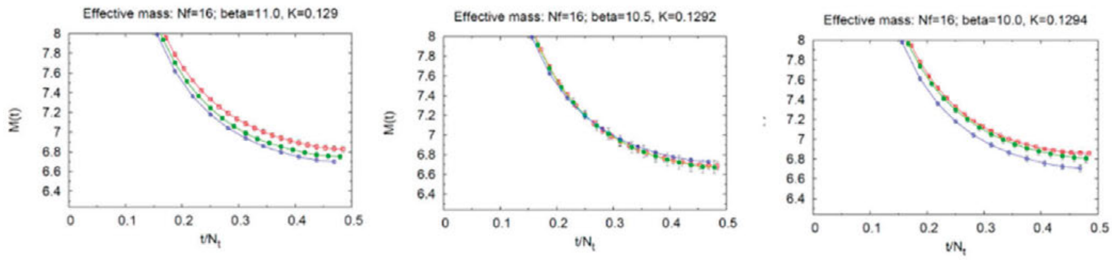

Fig.21. Scaled meson effective masses on $\mathbf{8^3} \times \mathbf{32}$ (blue), $\mathbf{12^3} \times \mathbf{48}$ (green) and $\mathbf{16^3} \times \mathbf{64}$ (red) lattices for $\boldsymbol{N_f}$=16. IR fixed point exits at $\boldsymbol{\beta}^{*}\sim$10.5.

1.3 Collaboration

In the TRG method the tensor defined at each site on a D-dimensional square lattice has 2D rank so that the computational cost of the TRG method, which is dominated by the contraction of the tensor indices, increases as the space-time dimension increases. For the analysis of four-dimensional models we need to perform a parallelization of the program. This is achieved in collaboration with applied mathematicians and computer scientists in Division of High Performance Computing Systems. We have successfully developed parallel programs for the Higher Order TRG (HOTRG) and the Anisotropic TRG (ATRG) methods, which are improved versions of the TRG method. These programs have contributed to the discovery of first-order phase transition in four-dimensional Ising model.

We have constructed ILDG (International Lattice Data Grid) and JLDG (Japan Lattice Data Grid) in collaboration with Grid and Network group in Division of High Performance Computing System. The former is to share gauge configurations among worldwide particle physics researchers through the internet and the latter for the domestic data sharing. Their operation started in 2007 and 2008, respectively. The more detailed description is provided in PART I of this report. The 2+1 flavor QCD gauge configurations generated in the PACS-CS project were uploaded on ILDG and widely used by particle physics researchers in foreign countries. We also plan to upload the 2+1 flavor QCD gauge configurations generated on the K computer in the near future.

As described in PART I of this report, the Joint Institute for Computational Fundamental Science (JICFuS) is a joint eight research organization including the Center for Computational Sciences (CCS) in University of Tsukuba. JICFuS has three major objectives. Firstly, all the organizations collaboratively provide researchers support for improving the algorithms and the computational techniques. Secondly, JICFuS serves as a place for computational fundamental scientists and computer scientists to interact and actively exchange ideas on a routine basis. Thirdly, we will promote collaborative interdisciplinary research between computational fundamental scientists in particle physics, nuclear physics and astrophysics, mediated by computer systems.

1.4 Future Plan

The current main project of PACS Collaboration is the master-field simulation. We are generating "PACS10" gauge configurations at the physical point on $(>10\ \mathrm{fm})^4$ lattice with the choice of three lattice spacings in 2+1 flavor QCD. These gauge configurations are dedicated to controlling three major systematic errors in lattice QCD: extrapolation in terms of quark masses, finite volume effect, and finite lattice spacing effect. So far we have finished generating two sets of gauge configurations of (lattice spacing, lattice size)=(0.085 fm, 128^4) and (0.065 fm, 160^4). The generation of the third set of gauge configurations with a finer lattice spacing is ongoing choosing a parameter set of (lattice spacing, lattice size)=(0.041fm, 256^4). With the use of a subset of PACS10 gauge configurations we have already obtained encouraging physics results: the kaon form factors in semileptonic decay, the nucleon form factors and the HVP contribution in $g-2$. In addition, we are now calculating the proton decay matrix elements. Once we finish the generation of the third set of gauge configuration, we perform a continuum extrapolation of the physical quantities at the three lattice spacings and make the systematic error due to the finite lattice spacing under control.

Another major research target is the study of the dynamics of QCD at finite temperature and finite density. There are three research directions in our group. The first one is to investigate the phase diagram in 3, 2+1 and 4 flavor QCD at finite temperature. Although we have mainly focused on the 3 flavor case so far, we plan to extend the analysis to the 2+1 and 4 flavor cases in the next step. The second one is to study the thermodynamics of QCD with the gradient flow. We have shown that the gradient flow method works well in calculating the equation of state in 2+1 flavor QCD with slightly heavy u, d quarks and approximately physical s quark. The next plan is to extend the study to 2+1 flavor QCD at physical u, d, s quarks. The third one is the systematic study of the thermodynamics of QCD with the Kogut-Susskind quarks around the physical point. This research direction is pursued in collaboration with the HotQCD group consisting of researchers mainly at Bielefeld University and BNL.

Application of TN scheme to particle physics is an encouraging new research subject. The TRG method, which is one of the TN schemes, has fascinating advantages: (i) no sign problem and no complex action problem, (ii) logarithmic volume dependence of computational cost,

(iii) direct treatment of Grassmann numbers, (iv) direct measurement of the partition function itself. We have confirmed the above features by successfully applying the TRG method to the analyses of various types of two-dimensional models. We have already started to perform an analysis of the four-dimensional models with the TRG method.

1.5 Publications

Journal Papers (refereed)

1. PACS Collaboration: Junpei Kakazu, Ken-ichi Ishikawa, Naruhito Ishizuka, Yoshinobu Kuramashi, Yoshifumi Nakamura, Yusuke Namekawa, Yusuke Taniguchi, Naoya Ukita, Takeshi Yamazaki, and Tomoteru Yoshié, “Kl3 form factors at the physical point on (10.9 fm)^3 volume”, arXiv:1912.13127[hep-lat] , to appear in Phys. Rev. D.
2. Daisuke Kadoh, Yoshinobu Kuramashi, Yoshifumi Nakamura, Ryo Sakai, Shinji Takeda, and Yusuke Yoshimura, “Investigation of complex $\phi 4$ theory at finite density in two dimensions using TRG”, JHEP 2002, ref.161 (2020).
3. Yoshinobu Kuramashi and Yusuke Yoshimura, “Tensor renormalization group study of two-dimensional U(1) lattice gauge theory with a θ term”, JHEP 2004, ref.089 (2020).
4. PACS Collaboration: K.-I. Ishikawa, N. Ishizuka, Y. Kuramashi, Y. Nakamura, Y. Namekawa, E. Shintani, Y. Taniguchi, N. Ukita, T. Yamazaki, and T. Yoshié, “Finite size effect on vector meson and baryon sectors in 2+1 flavor QCD at the physical point”, Phys. Rev. D100, ref.094502 (2019).
5. Shinichiro Akiyama, Yoshinobu Kuramashi, Takumi Yamashita, and Yusuke Yoshimura, “Phase transition of four-dimensional Ising model with higher-order tensor renormalization group”, Phys. Rev. D100, ref.054510 (2019).
6. Yoshinobu Kuramashi and Yusuke Yoshimura, “Three-dimensional finite temperature Z2 gauge theory with tensor network scheme”, JHEP 1908, ref.023 (2019).
7. PACS Collaboration: E. Shintani and Y. Kuramashi, “Hadronic vacuum polarization contribution to the muon g−2 with 2+1 flavor lattice QCD on a larger than (10 fm)^4 lattice at the physical point”, Phys. Rev. D100, ref.034517 (2019).
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11. HotQCD Collaboration: A. Bazavov, H.-T. Ding, P. Hegde, O. Kaczmarek, F. Karsch, N. Karthik, E. Laermann, Anirban Lahiri, R. Larsen, S.-T. Li, Swagato Mukherjee, H. Ohno, P. Petreczky, H. Sandmeyer, C. Schmidt, S. Sharma and P. Steinbrecher, "Chiral crossover in QCD at zero and non-zero chemical potentials", Phys. Lett. B795, ref.15 (2019).
12. HotQCD Collaboration: H.-T. Ding, P. Hegde, O. Kaczmarek, F. Karsch, Anirban Lahiri, S.-T. Li, Swagato Mukherjee, H. Ohno, P. Petreczky, C. Schmidt, and P. Steinbrecher, "Chiral Phase Transition Temperature in (2+1)-Flavor QCD", Phys. Rev. Lett. 123, ref.062002 (2019).
13. HotQCD Collaboration: A. Bazavov, S. Dentinger, H.-T. Ding, P. Hegde, O. Kaczmarek, F. Karsch, E. Laermann, Anirban Lahiri, Swagato Mukherjee, H. Ohno, P. Petreczky, R. Thakkar, H. Sandmeyer, C. Schmidt, S. Sharma, and P. Steinbrecher, "Meson screening masses in (2+1)-flavor QCD", Phys. Rev. D100, ref.094510 (2019).
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16. PACS Collaboration: Naoya Ukita, Ken-Ichi Ishikawa, and Yoshinobu Kuramashi, “Utility of geometry in lattice QCD simulations”, Phys. Rev. D98, ref.014515 (2018).
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18. PACS Collaboration: Ken-Ichi Ishikawa, Yoshinobu Kuramashi, Shoichi Sasaki, Natsuki Tsukamoto, Akira Ukawa, and Takeshi Yamazaki, “Nucleon form factors on a large volume lattice near the physical point in 2+1 flavor QCD”, Phys. Rev. D 98, ref.074510 (2018).
19. Takeshi Yamazaki and Yoshinobu Kuramashi, “Reply to “Comment on ‘Relation between scattering amplitude and Bethe-Salpeter wave function in quantum field theory’”, Phys. Rev. D 98, ref.038502 (2018).
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23. Yuya Shmizu and Yoshinobu Kuramashi, "Berezinskii-Kosterlitz-Thouless Transition in Lattice Schwinger Model with One-Flavor of Wilson Fermion", Phys. Rev. D 97, ref.034502 (2018).
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Books

Awards

1.6 Grants

1. Yoshinobu Kuramashi (CI), MEXT “Exploratory Challenge on Post-K computer” (PI: Momoji Kubo), FY2016-FY2019, 67,155,000 yen
2. Yoshinobu Kuramashi (PI), JSPS Grant-in-Aid for Scientific Research (B), FY2015-FY2017, 16,770,000 yen
3. Yoshinobu Kuramashi (CI), JST CREST (PI: Tetsuya Sakurai), FY2011-FY2015, 7,653,100 yen
4. Kazuyuki Kanaya (PI), JSPS Grant-in-Aid for Scientific Research (C), FY2019-FY2021, 4,290,000 yen
5. Kazuyuki Kanaya (PI), JSPS Grant-in-Aid for Scientific Research (C), FY2015-FY2018, 4,550,000 yen
6. Naruhito Ishizuka (PI), JSPS Grant-in-Aid for Scientific Research (B), FY2015-FY2017, 14,430,000 yen
7. Yusuke Taniguchi (PI), JSPS Grant-in-Aid for Scientific Research (C), FY2018-FY2022, 4,550,000 yen
8. Yusuke Taniguchi (PI), JSPS Grant-in-Aid for Scientific Research (C), FY2010-FY2014, 3,250,000 yen
9. Takeshi Yamazaki (PI), JSPS Grant-in-Aid for Scientific Research (B), FY2019-FY2022, 17,030,000 yen
10. Takeshi Yamazaki (PI), JSPS Grant-in-Aid for Young Scientists (A), FY2016-FY2018, 23,660,000 yen
11. Takeshi Yamazaki (PI), JSPS Grant-in-Aid for Young Scientists (B), FY2013-FY2015, 4,030,000 yen
12. Naoya Ukita (PI), JSPS Grant-in-Aid for Challenging Exploratory Research, FY2016-FY2018, 3,510,000 yen
13. Naoya Ukita (PI), JSPS Grant-in-Aid for Young Scientists (B), FY2012-FY2014, 4,420,000 yen
14. Yusuke Namekawa (PI), JSPS Grant-in-Aid for Scientific Research (C), FY2015-FY2017, 2,990,000 yen
15. Yusuke Namekawa (PI), JSPS Grant-in-Aid for Scientific Research (C), FY2012-FY2014, 2,990,000 yen

2 Division of Astrophysics

2.1 Overview

In the astrophysics group, we have explored merger of black holes, first generation objects, formation and evolution of galaxies, active galactic nuclei, accretion and outflows around black holes, missing satellite problem on dark haloes, large-scale galactic winds, cluster of galaxies, large-scale structures, and early universe. Also, we have diversified the research field into multidisciplinary computational sciences, which include Computational Astrobiology (CAB) and computational optical bioimaging in "Computational Medical Science (CMS)". In addition, we have promoted the collaboration with the Division of High Performance Computing Systems to construct the Cygnus system (see Part I for more details).

2.2 Research Results

1) Mergers of Accreting Multiple BHs Leading to SMBH Formation in Galactic Nuclei

Recent gravitational-wave (GW) measurement of black hole (BH) spins by aLIGO favors misalignment with the orbital angular momentum, which prefers a formation scenario where no spin alignment process is present. As a possibility, we consider BH mergers via "chance meeting" promoted in a multiple BH system under the gas-rich environments in galactic nuclei. For the purpose, we simulate orbits of multiple BHs in gas-rich environments with a post-

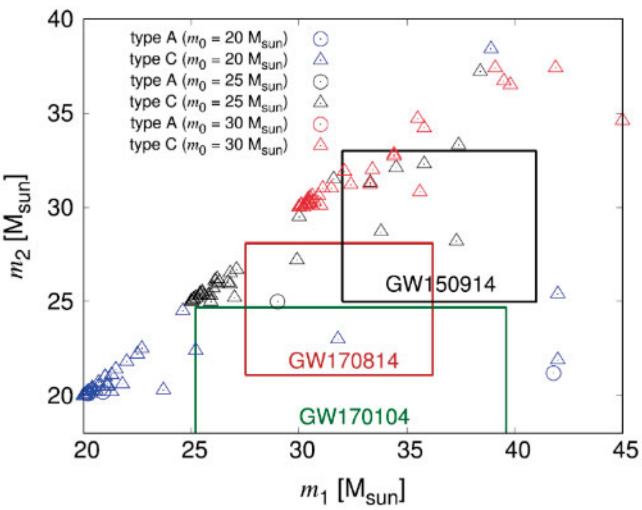

Figure 1: BH masses in a merging binary just before the first merger, and comparison to the GW events.

Newtonian N-body scheme, incorporating gas accretion, dynamical friction, and GW emission. As a result, we find that gas dynamical friction effectively promotes a three-body interaction of BHs in dense gas of $n_{gas} \gtrsim 10^6$ cm^{-3}, so that BH mergers can take place within 30 Myr. This scenario predicts an isotropic distribution of spin tilts (Tagawa & Umemura 2018). The results are concordant with the observations by aLIGO (Fig.1).

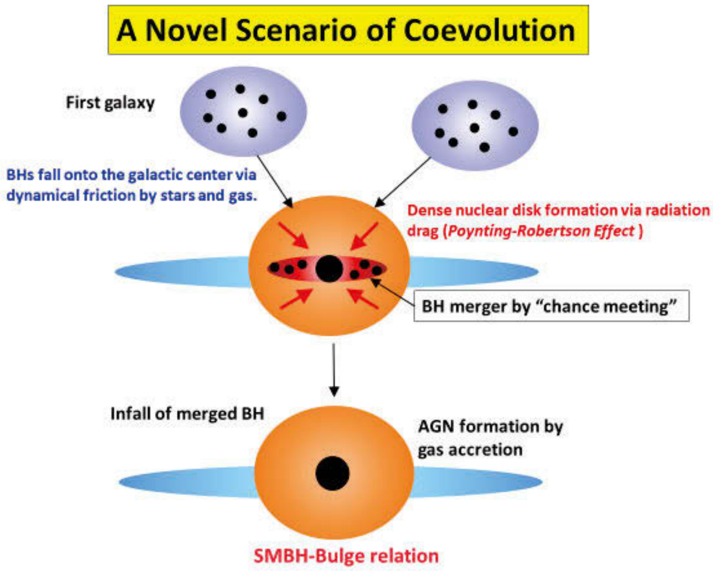

Figure 2: Scenario for the coevolution of SMBHs and galaxies, incorporating BH mergers.

Based on these results, we propose a novel scenario for the establishment of supermassive black holes (SMBH)-to-galactic bulge relation. Previously, Umemura (2001) proposed a radiation-hydrodynamic mechanism to build up an SMBHs, where the radiation drag by bulge stars extracts angular momentum from interstellar gas through "Poynting-Robertson effect", and thus allows the gas to accrete onto the galactic center. In this scenario, the SMBH-to-bulge mass ratio is predicted to be 0.3ε–0.5ε, where ε is the energy conversion efficiency for nuclear fusion of hydrogen to helium, i.e., 0.007. Combined with BH merger in a dense nuclear disk, a novel scenario for the coevolution of SMBHs and galaxies is as follows. First, seed BHs fall onto the galactic center via dynamical friction by stars and gas. Simultaneously, a dense nuclear disk forms via radiation drag (Poynting-Robertson effect). The seed BHs accompanied with gas accretion merge into a larger BH via "chance meeting" in a nuclear disk and the merged BH falls onto the galactic center. Then, AGN is activated by accretion of the gas disk. After the AGN phase, the SMBH-to-galactic bulge relation is established (Fig. 2).

2) Distribution of Heavy Elements Originating from Pop III Stars

We consider a possible way to approach the evidence of Pop III stars through the observation of the heavy elements ejected by the supernova explosions of massive Pop III stars. To the end, we investigate the distribution of metals provided by massive Population III (Pop III) stars in the cosmological volume at z~3, using a cosmological N-body simulation in which a model of Pop III star formation is implemented (Kirihara et al. 2020). Owing to the simulation, we can choose minihaloes where Pop III star formation occurs at z > 10 and obtain the spatial distribution of the

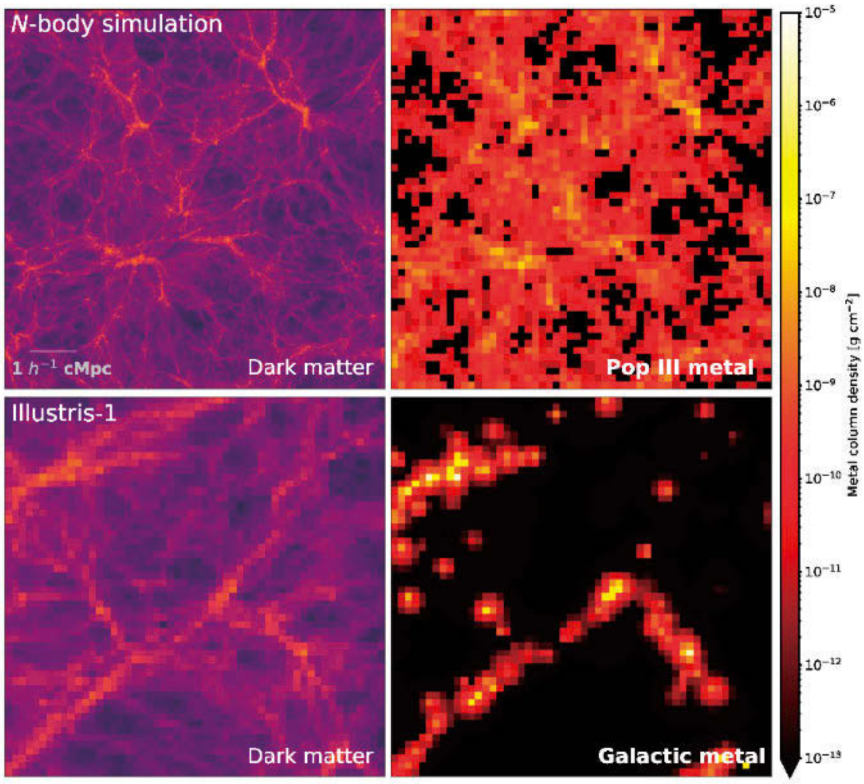

Figure 3: Top: Column density distribution of dark matter (left) and Pop III originated metals (right) obtained by the cosmological N-body simulation at z =3. Bottom: Column density distribution of darkmatter (left) and galactic metals (right) obtained by the Illustris-1 simulation.

metals at lower redshifts. To evaluate the amount of heavy elements provided by Pop III stars, we consider metal yield of pair-instability or core-collapse supernovae (SNe) explosions of massive stars. By comparing our results to the Illustris-1 simulation, we find that heavy elements provided by Pop III stars often dominate those from galaxies in low-density regions (Fig. 3). The median value of the volume averaged metallicity is $Z \sim 10^{-4.5}$-10^{-2} $Z_{\odot}$ at the regions.

3) Observational Universalities of Dark Matter Halos in Less Massive Galaxies

Recent observations around less massive galaxies have revealed interesting universal properties of dark matter halos (DMHs). For example, DMHs have common enclosed masses within 300 pc proposed by Strigari et al., and Kormendy & Freeman reported DMHs having almost identical central surface densities. Ogiya & Mori (2014) investigate whether a scenario where cuspy haloes transform into cores by dynamical processes can also explain their universal properties in DMHs. In this study, we show that our model of a cusp-to-core transformation in DMHs naturally reproduces the Kormendy-Freeman relation and that Strigari relation follows from the Kormendy-Freeman relation for dwarf galaxies. Moreover, it is shown that the central densities of DMHs with core conserve valuable information about their formation epochs.

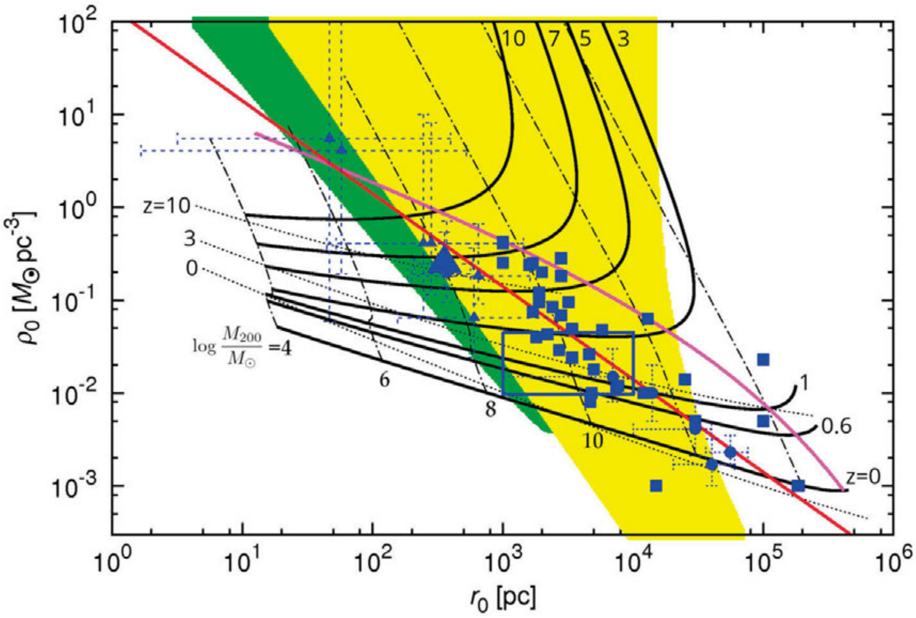

Figure 4: Diagram core radius r_0 vs. core density ρ_0, taken from Ogiya and Mori, MNRAS, 440, 71 (2014). Respective points show the parameters of Burkert profile, ρ_0 and r_0, obtained by observations. Triangles, squares and circles represent the data from Salucci et al. (2012), Spano et al. (2008) and Donato et al. (2009), respectively. Red line is the scaling relation between ρ_0 and r_0 proposed by Salucci et al. (2012). The place embraced by blue box corresponds to the results of Burkert (1995). Solid and dotted black lines show the results of our analysis applying the c(M, z) proposed by Prada et al. (2012) and Macci`o et al. (2008), respectively.

4) Observational Predictions for a Wandering Massive Black Hole in the Halo of M31

Galaxies and massive black holes presumably grow via galactic merging events and subsequent black hole coalescence. As a case study, Kawaguchi, Saito, Miki & Mori (2014) investigate the merging event between the M31 and a satellite galaxy. We compute the expected observational appearance of the massive black hole that was at the center of the satellite galaxy prior to the merger and is currently wandering in the M31 halo. We demonstrate that a radiatively inefficient accretion flow with a bolometric luminosity of a few tens of solar luminosities develops when Hoyle-Lyttleton accretion onto the black hole is assumed. We compute the associated broadband spectrum and show that the radio band (observable with EVLA, ALMA, and the Square Kilometre Array) is the best frequency range in which to detect the emission. We also evaluate the mass and the luminosity of the stars bound by the wandering black hole and find that such a star cluster is sufficiently luminous that it could correspond to one of the star clusters found by the PAndAS survey. The discovery of a relic massive black hole wandering in a galactic halo will provide a direct means of investigating in detail the coevolution of galaxies and black holes. It also means a new population of black holes (off-center massive black holes) and offers targets for clean black hole imaging that avoid strong interstellar scattering in the centers of galaxies.

5) The Nature of the Progenitor of the M31 North-western Stream

Kirihara, Miki & Mori (2017) examine the nature, possible orbits and physical properties of the progenitor of the north-western stellar stream (NWS) in the halo of the M31. The progenitor is assumed to be an accreting dwarf galaxy with globular clusters (GCs). It is, in general, difficult to determine the progenitor's orbit precisely because of many necessary parameters. Recently, Veljanoski et al. reported five GCs whose positions and radial velocities suggest an association with the stream. We use these data to constrain the orbital motions of the progenitor using test-particle simulations. Our simulations split the orbit solutions into two branches according to whether the stream ends up in the foreground or in the background of M31. Upcoming observations that will determine the distance to the NWS will be able to reject one of the two branches. In either case, the solutions require that the pericentric radius of any possible orbit be over 2 kpc. We estimate the efficiency of the tidal disruption and confirm the consistency with the assumption for the progenitor being a dwarf galaxy. The progenitor requires the mass $\gtrsim 2 \times 10^6\ M_\odot$ and half-light radius $\gtrsim$ 30 pc. In addition, N-body simulations successfully reproduce the basic observed features of the NWS and the GCs' line-of-sight velocities.

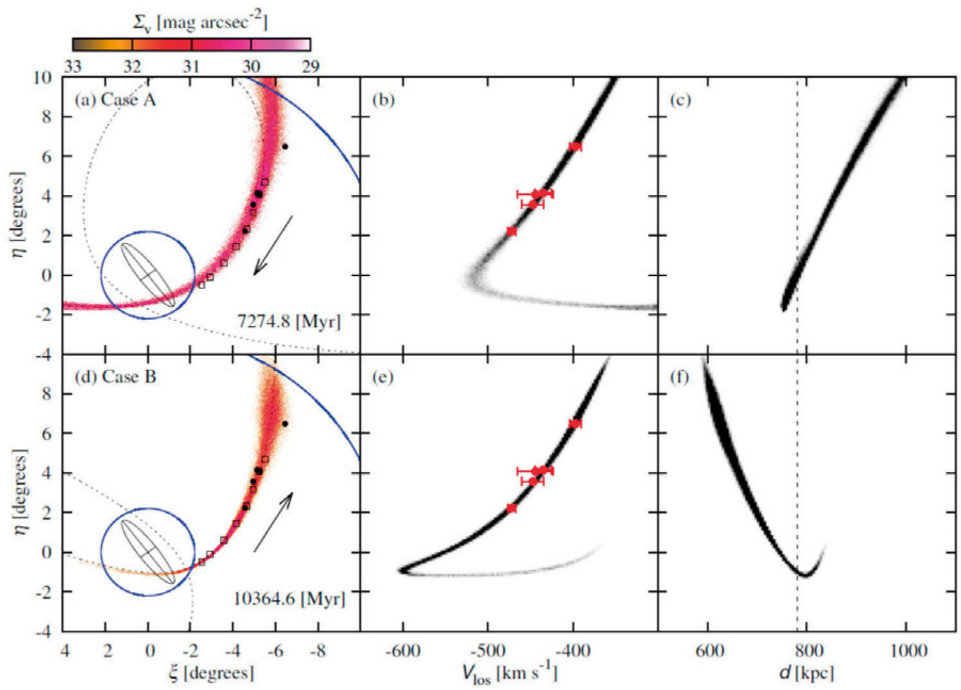

Figure 5: Spatial distribution of the simulated NWS in sky coordinates taken from Kirihara, Miki and Mori, MNRAS, 469, 3390 (2017). The streams move in the directions of the arrows. The ellipse traces M31's disc, and blue circles trace a radius of 30 kpc and 150 kpc from M31's centre. Filled black circles mark the positions of the observed GCs aligned with the NWS.

6) Transonic Galactic Outflows in a Dark Matter Halo with a Central Black Hole

Igarashi, Mori & Nitta (2017) investigate polytropic transonic solutions of spherically symmetric and steady galactic winds in the gravitational potential of a DMH with an SMBH. The solutions are classified in terms of their topological features, and the gravitational potential of the SMBH adds a new branch to the transonic solutions generated by the gravity of the DMH. The topological types of the transonic solutions depend on the mass distribution, the amount of supplied energy, the polytropic index γ and the slope α of the DMH mass distribution. When α becomes larger than a critical value αc, the transonic solution types change dramatically. Further, our model predicts that it is possible for a slowly accelerating outflow to exist, even in quiescent galaxies with small γ. This slowly accelerating outflow differs from those considered in many of the previous studies focusing on supersonic outflows in active star-forming galaxies. In addition, our model indicates that outflows in active star-forming galaxies have only one transonic point in the inner region ~(0.01 kpc). The locus of this transonic point does not strongly depend on γ. We apply the polytropic model incorporating mass flux supplied by stellar components to the Sombrero galaxy, and conclude that it can reproduce the observed gas density and the temperature distribution well. This result differs significantly from the isothermal model, which requires an unrealistically large mass flux. Thus, we conclude that the polytropic model is more realistic than the isothermal model, and that the Sombrero galaxy can have a slowly accelerating outflow.

7) Super-Eddington Accretion Flows and Jets around Black Holes

We perform general relativistic radiation-magnetohydrodynamic simulations of supercritical accretion disks and jets around black holes (BHs). It is found that the strong radiation pressure supports the geometrically thick disks and the radiatively driven jets are launched from the disk surface via the radiation pressure force. The jet velocity becomes about 30-50% of the speed of light. The matter is not accelerated anymore due to radiation drag. Our simulations also reveal

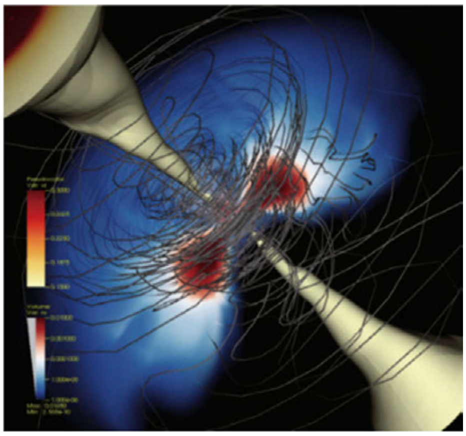

Figure 6: Super-Eddington accretion disk (red) and jets (white) obtained by general relativistic radiation magnetohydrodynamics simulations. Gray thin lines indicate magnetic field lines.

that the temperature of the disk around Kerr BH is higher than that around Schwarzschild BH. It is thought to be caused by the Blandford-Znajek effect, by which the rotation energy of the BH is extracted through the magnetic fields. Indeed, the outward Poynting Flux is enhanced around Kerr BH.

8) Modeling of Ultraluminous X-ray Sources; Super-Eddington Accretion onto Neutron Stars

We perform the general relativistic radiation magnetohydrodynamics simulations of the supercritical accretion onto magnetized neutron stars (NSs) in order to reveal the energy production mechanism of the ultraluminous X-ray sources (ULXs). The disk is truncated by the strong dipole magnetic fields of the NSs. Thus, the disk matter moves along the magnetic field lines and falls around the magnetic poles of the NS, forming the accretion columns. By the radiation hydrodynamics simulations which are focusing on the accretion columns, we find that the radiation energy is drastically enhanced within the accretion column via the shock. However, radiation pressure does not prevent gas from falling down in the accretion column since most photons escape from the side wall of the column (the luminosity of the side wall of the columns exceed the Eddington luminosity). This is why steady supercritical accretion is realized. Our results imply that the observed luminosity changes periodically with the rotation of NSs. Such features are consistent with the recent observations of pulsed-ULXs. Our calculations support the hypothesis that pulsed-ULX is powered by the supercritical column accretion flows onto the magnetized NSs.

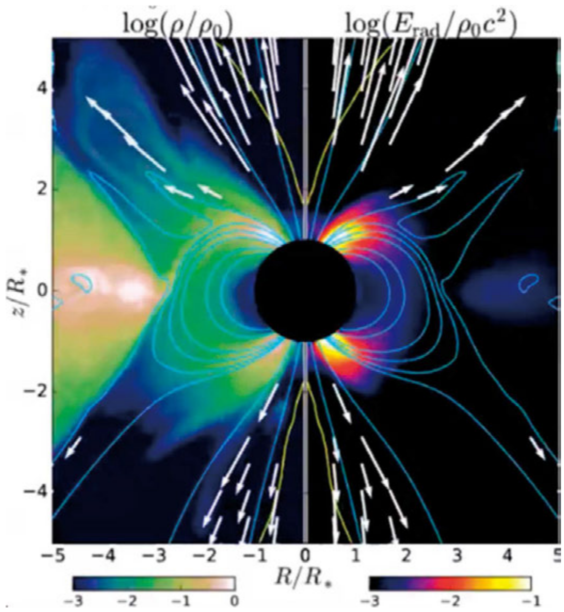

Figure 7: Profiles of the density (left half) and the radiation energy density (right half) of the super-Eddington accretion flows around a magnetized neutron star. The accretion disk is truncated and the accretion columns appear at around the magnetic poles.

9) Disk Winds from the Near-Eddington Accretion Disk around Black Holes

We investigate the disk wind launching from the near-Eddington accretion disks around black holes (BHs) using radiation hydrodynamics simulations. As a result, it is found that when a central object is a supermassive black hole (SMBH), the disk winds are blown away from the regions of ~100 gravitational radii. This disk wind is accelerated by the radiation force due to spectral lines (line force) and the wind velocity is about 10% of the speed of light. The wind matter includes the heavy ions in low-ionization state so that it is thought to produce the blue-shifted absorption features in X-ray band. Indeed, since the velocity, column density, and ionization degree are consistent with those of the estimation based on the observed absorption features, the disk wind driven by the line force is believed to be the origin of the ultrafast outflows (so-called UFOs). In addition, when a central celestial object is a stellar mass black hole, the gas heated by X-ray irradiation blows out by the gas pressure and radiation pressure, producing the disk wind. The launching radius of the wind is about 10,000 gravitational radii. As a result of the spectrum calculation, our model nicely fits the observed iron absorption lines.

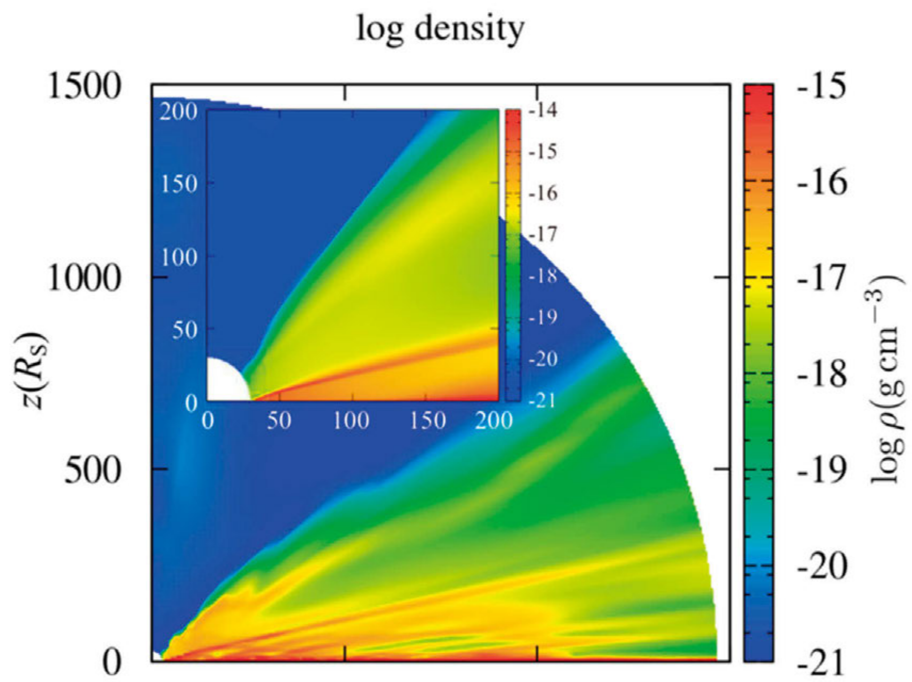

Figure 8: Time averaged density map of the disk wind launched from the near-Eddington accretion disk around the supermassive black hole. The funnel-shaped disk wind appears, in which dense matter is accelerated outward with an opening angle of 70–80◦ and with 10% of the light speed.

10) Radiative Properties of High-redshift Galaxies

Combining cosmological hydrodynamics simulations and radiative transfer calculations, we investigate the observational properties of galaxies in the early Universe. We show that Lyman-alpha and Lyman continuum photons escape from low-mass haloes efficiently and contribute to the cosmic reionization. As the halo mass increases, dusty gas covers star-forming regions. As a result, massive galaxies become bright at infrared wavelengths because of dust thermal emission. Sub-millimeter fluxes from the simulated galaxies show ~0.1 mJy at 850-micron meter in the observed frame, which nicely matches high-redshift galaxies observed by Atacama Large Millimeter/Submillimeter Array. This transition occurs at the halo mass around 1012 M⊙. In the massive galaxies, dusty clouds keep distributing around star-forming regions against supernova feedback. We also show that UV continuum radiation from galaxies even at $z \sim 12$ can be observed by James Webb Space Telescope.

11) Growth of First Galaxies with Supernova Feedback

Using cosmological hydrodynamics simulations with zoom-in initial conditions, we study the formation mechanism of first galaxies. We focus on three different galaxies with the halo masses Mhalo = 2.4×1010, 1.6×1011, and 0.7×1012 M⊙ at z=6. We find that star formation occurs intermittently due to supernova feedback at $z > 10$, and then it proceeds more smoothly as halo's gravitational potential well becomes deep. The star burst and quench processes repeat with the time scale of 10 Myr which is shorter than the halo dynamical time. In addition, we show that galactic morphology sensitively depends on the star formation and feedback models. Gas disk is destroyed in the fiducial run, while galaxies in the case of low-star formation efficiency model keep hosting galactic disks for a long time. We show that the simulated galaxies in star-burst phases reproduce the physical properties of observed Lyman-alpha emitting galaxies at $z > 6$, e.g., star formation rate and stellar mass.

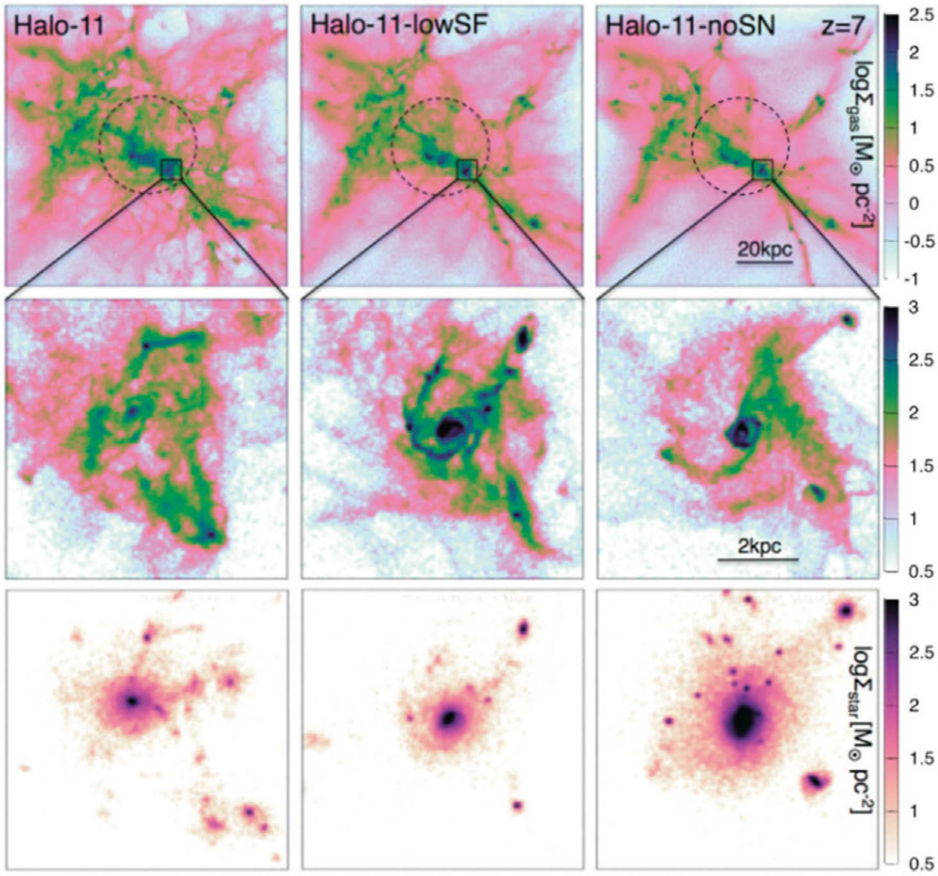

Figure 9. Column density of gas in the simulated galaxies at z=7. The top panels show the filamentary network of gas distribution on a scale of physical scale 100 kpc, and dashed circles show the virial radius ~ 18 kpc. The middle panels show the zoom-in view of the most massive galaxy in the halo with a scale of physical 7 kpc. The lower panels represent the stellar surface density with the same logarithmic scale as the middle panels. The galaxies have quite different morphologies depending on the treatment of star formation and stellar feedback (Yajima et al. 2017, ApJ, 846, 30).

12) Vlasov Simulations for Self-Gravitating System and Magnetized Plasma

As an alternative to standard N-body simulations of collisionless self-gravitating systems, we devise a new approach that follows the time evolution of distribution function of matter in the six-dimensional phase space by directly solving the collisionless Boltzmann equation (or Vlasov equation) in a finite volume manner. Since this approach (hereafter Vlasov simulation) requires a very large amount of memory to map the six-dimensional phase space, the number of mesh grids and the spatial resolution is still limited by the available amount of memory. Therefore, it is necessary to devise spatially higher order numerical schemes to increase the spatial resolution effectively. We develop a set of numerical schemes for solving the Vlasov equation that has spatially fifth- and seventh-order accuracy and preserves the monotonicity and the positivity of numerical solutions. These schemes are verified with various numerical tests of collisionless self-gravitating systems. We find that they are remarkably good at solving rigid body rotation with very small numerical dissipation, and can be applied to Vlasov simulations of astrophysical magnetized plasma.

13) Dynamical Effect of Cosmological Relic Neutrinos on Large-Scale Structure Formation

After the discovery of neutrino oscillation, it is well understood that cosmological relic neutrinos are currently non-relativistic and they have a dynamical impact on the large-scale structure in the universe. We investigate the dynamical effect of massive neutrinos on large-scale structure formation by performing a set of numerical simulations in which the dynamics of massive neutrinos is simulated using a Vlasov simulation while that of CDM component is solved with the conventional N-body method. Adopting the Vlasov approach enables us to perform a noiseless simulation of massive neutrinos unlike conventional N-body simulations, and to accurately compute the free streaming effect of massive neutrinos.

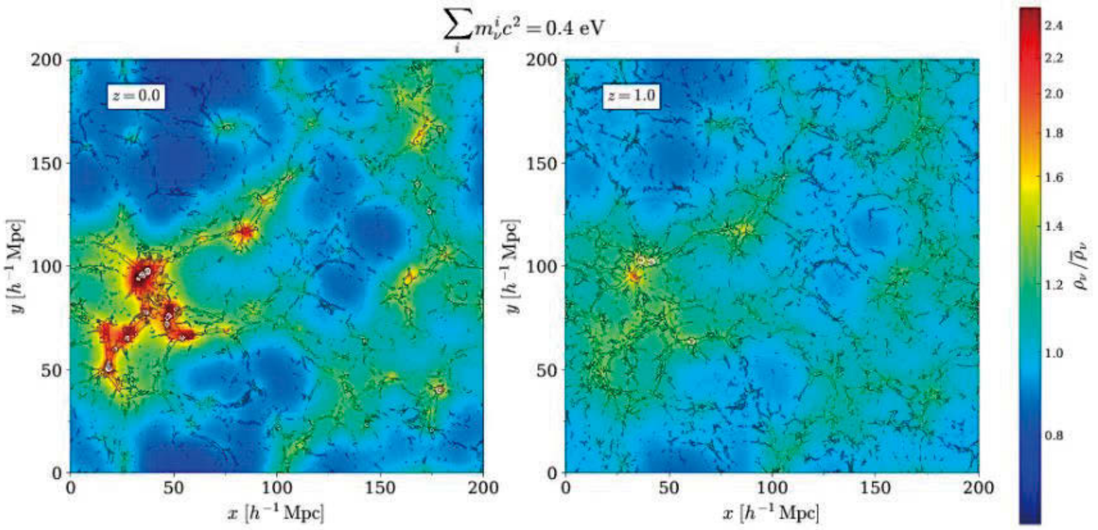

Figure 10. Maps of density field of CDM (contour) and neutrinos at redshift of z=0 and 1 obtained with our numerical simulation.

14) Detectability of Warm-Hot Intergalactic Medium through Hyperfine Structure Transition of Heavy Elements

It is well known that most of the cosmic baryon is in the form of sparse plasma with a temperature of 10^5 to 10^7 K, known as "Warm-Hot Intergalactic Medium" (hereafter WHIM). Despite recent extensive searches for WHIM, a significant fraction of WHIM is still yet to be identified. So far, WHIM has been detected as UV/X-ray absorption lines of heavy elements (O, C, Ne) along the lines of sight toward background bright sources. We investigate another observational method to detect WHIM in radio bands, in which absorption features of hyperfine structure transition of nitrogen are targeted, find that next generation radio interferometer such as Square Kilometer Array (SKA) and ngVLA can detect WHIM with this alternative method.

15) Jet-, Wind- and Radiation-Driven AGN Feedback

Active galactic nucleus (AGN) feedback is thought to be responsible for the coevolution of galaxy and central supermassive black hole that manifests itself in, e.g., the tight relationship between galaxies' stellar content and black hole mass, but the mechanisms and efficiencies with which AGN regulate the conditions of the interstellar medium (ISM) are not well understood. Our suites of high-resolution, large-scale, idealized relativistic hydrodynamical simulations of the interaction of AGN winds, jets, and radiation with the ISM have shed light on the way energy is imparted to the ISM and how star-formation is consequently affected. We paid particular attention to the modelling of the ISM on whose properties the feedback efficiencies depend strongly.

An important outcome of our simulations, which goes against the conventional understanding of how AGN feedback works, is that gas ejection from galaxies is very inefficient, even for the most powerful AGN. This is partly because the porosity of the ISM vents the energy contained in the AGN driven bubbles. In our simulations, individual clouds are well resolved, and strong radiative cooling behind shocks driven into the clouds creates dense layers that protect the clouds from ablation.

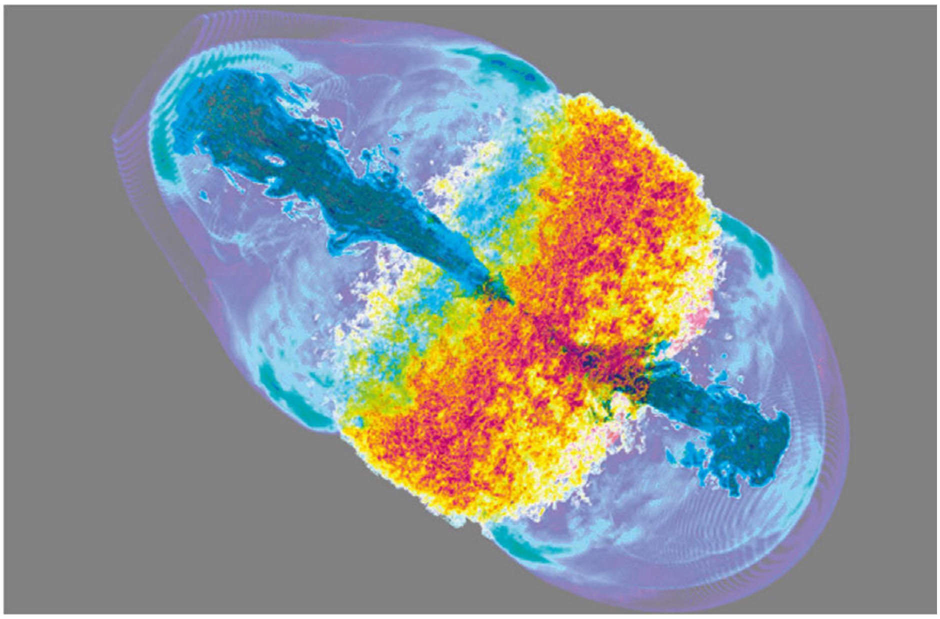

Figure 11: Volume render of a simulation of a relativistic jet (blue) interacting with the disc of a gas-rich galaxy. The jet drives shock waves into the gaseous disc and temporarily induces star-formation, before the jet plasma percolating through the porous interstellar medium of the disc begins to strongly disperse the gas, reducing star-formation.

For AGN jets, we explored the dependence of jet-ISM interactions on the jet tilt angle relative to the galactic disc. In general, a higher tilt angle results in stronger interactions, but the quantitative differences are complex. Turbulence is induced in different parts of the galaxy by the streams of jet plasma percolating through the porous ISM. In most cases, a phase of positive feedback, in which star-formation is induced, is followed by a longer period of negative feedback in which star-formation is reduced.

We performed simulations of AGN radiation driven outflows on galaxy scales. As was the case for jets, the efficiency of feedback depended on the ISM conditions, in particular, the size-scale of clouds. Infrared, optical, and UV photons all played a role in providing momentum boosts of a few tens, as is commonly seen in outflows of high-redshift AGN, with the main source of momentum boost coming from the multiply scattering infrared photons.

We have compared jet driven AGN feedback with radiation driven AGN feedback for the same ISM conditions and found that for both strong and weak AGN powers, jets are more efficient in driving out mass and accelerating dense gas. An indicator that may be used to distinguish the AGN driver is the density-velocity correlation of accelerated gas; when gas is accelerated by jets (that is, mechanical feedback), the density and velocity show an anti-correlation during the first Myr, while for the case of radiation-driven feedback, the density and velocity are correlated. The physical interpretation is that in mechanical feedback, the outer layer of clouds experiences stronger acceleration through ablation than the inner layers, while in the case of radiation-driven feedback, the infrared photons penetrate into the dense inner layers of clouds depositing more momentum there than in the outer layers.

16) Confronting Simulations of AGN Jet Feedback with Observations

We have begun an extensive program of comparisons of AGN jet feedback with observations. Among the sources in which we have performed direct, quantitative comparisons are Hydra A, IC 5063, B2 0258+35, UGC 05771, 4C 31.04, and qualitative comparisons with NGC 1052, NGC 3079, 3C 326, 3C 293, and a sample of NLS1 as well as a sample of dust obscured galaxies harboring AGN.

Through a suite of simulations designed to investigate compact gas-rich young radio galaxies called GPS and CSS sources, we have been able to provide strong evidence that these sources are part of an evolutionary progression. We connected the spectral evolution of GPS sources to CSS sources to the propagation of the jet through the clumpy ISM and the resulting dispersion of the ionized gas that results in a decrease in the optical depth of the synchrotron radiation to free-free absorption.

17) Cloud destruction and Mixing in Astrophysical Flows

The dynamics of entrained outflows is a key physical mechanism in AGN feedback, starburst galaxies, and supernova-ISM interactions, and has been studied for decades, but the understanding of mixing processes is incomplete. In particular, the internal turbulent nature of the clouds has never been considered in theoretical work. How do the turbulent characteristics of clouds affect their stability and their disruption when embedded in astrophysical flows? We performed high-resolution MHD simulations of fractal and turbulent clouds embedded in supersonic astrophysical flows and studied the dependence of cloud survival, fragmentation and mixing on the degree of solenoidal versus compressive turbulence in the clouds. We found that compressive clouds compared to solenoidal clouds are 1) more confined, less accelerated, and have lower velocity dispersion; 2) are less prone to Kelvin-Helmholtz and Rayleigh-Taylor instabilities, so they survive longer; 3) less effective gas entrainment but more effective mass loading

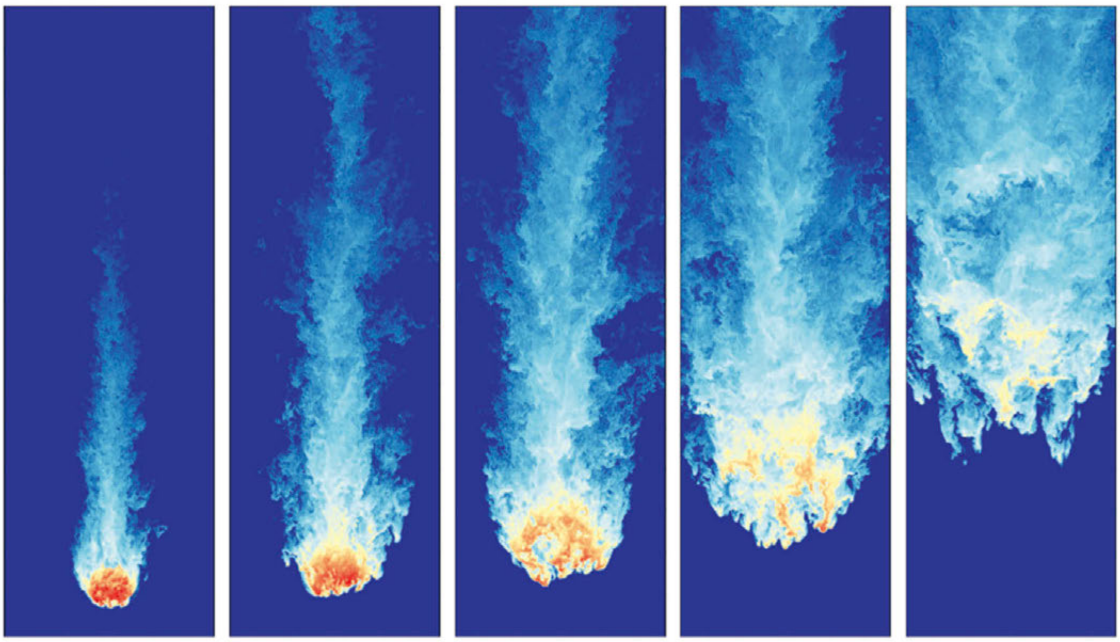

Figure 12: Midplane slices of the density evolution of turbulent clouds embedded in supersonic astrophysical flows. This example shows a cloud dominated by solenoidal turbulence, that is, vortices. Such clouds have shorter lifetimes than clouds dominated by compressive turbulence, presumably because the vortices quickly cascade to smaller scales, leading to faster dissipation of energy and expansion and mixing of the clouds.

18) Water Trail from Clouds to Protoplanetary Disks probed with Deuterium Fractionation

Water is one of the most important molecules in space, because a significant fraction of oxygen is present as water in the ISM, water is the raw material of planetary systems, and water is essential for life on Earth. We constructed a detailed model of water trail from its formation in molecular clouds to the delivery to protoplanetary disks, considering deuterium fractionation chemistry. For the first time, our model successfully reproduced the HDO/H2O ratio and the D2O/HDO ratio observed in the low-mass star-forming regions and measured in cometary ices, by starting the simulation from the formation of molecular clouds and by considering layered structure of ice mantles. We showed that (i) water is mostly formed in molecular clouds as ice, (ii) deuterated in cold denser cores, and (iii) delivered to protoplanetary disks without significant alteration. The results support the scenario that water in the solar system was inherited from the presolar cloud.

19) Mechanism of Nitrogen Isotope Fractionation

Nitrogen isotope fractionation (i.e., the $^{14}N/^{15}N$ ratio in molecules deviates from the elemental $^{14}N/^{15}N$ ratio) has been observed both in the ISM and in cometary coma in our solar system. The mechanism of the fractionation, however, was not understood. We proposed that nitrogen isotope fractionation occurs via the combination of isotope selective photodissociation of N2 and ammonia ice formation in molecular clouds. By performing astrochemical simulations, we showed that this mechanism can explain (i) the nitrogen isotope fractionation observed in the ISM and in cometary coma, and (ii) different fractionation patterns between hydrogen and nitrogen observed in them. We conducted an observational study to further test the proposed mechanism using the IRAM 30m telescope, and the observational result (N2D+ is depleted in 15N in a prestellar core) is consistent with our model prediction.

20) Chemistry in Protoplanetary Disks

We developed a detailed 2D axisymmetric model of the chemical structure of protoplanetary disks. The model includes both gas-phase and ice chemistry and turbulence mixing in the vertical direction, the last of which was found to affect the disk chemical structure significantly. The model has been used for various theoretical studies and interpretation of molecular line observations, including the first detection of complex organic molecules in protoplanetary disks. In addition, we recently performed new simulations that include both chemistry and dust evolution in protoplanetary disks. We found that models with low fragmentation velocity (the value appropriate for CO2 ice rather than water ice) are more consistent with the high-resolution ALMA observations of CO in a protoplanetary disk.

21) Theoretical Model of the Early Universe

We study the so-called Bubble Universe as a new scenario of the early Universe motivated by the context of string landscape, where our universe is produced by a new vacuum bubble embedded in an old bubble and these bubble universes have not only different cosmological constants, but also their own different gravitational constants. We have investigated these effects on the primordial curvature perturbations by different gravitational constants. In particular, the primordial curvature perturbation on superhorizon scales can be affected by the wall trajectory as the boundary effect. We showed the effect of gravitational constant in the exterior bubble universe can provide a peak like a bump feature at a large scale in a modulation of the power spectrum.

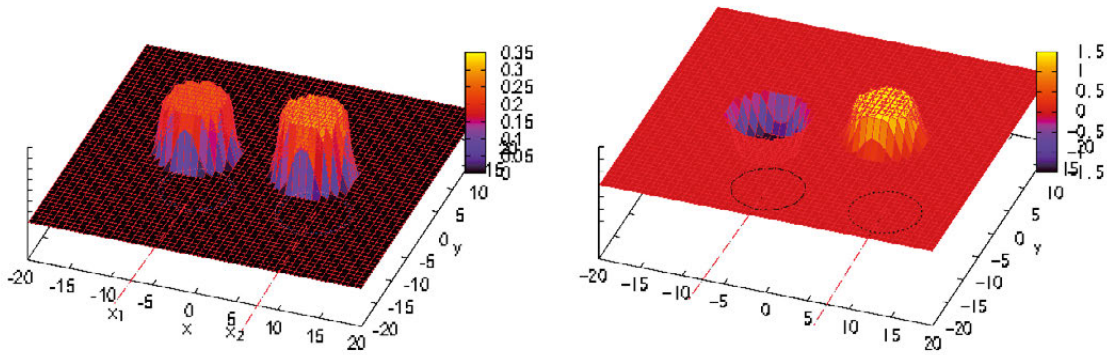

Figure 13: Snapshot of metric coefficient $A(x, y, t)$ (left) and field $\phi\,(x, y, t)$ (right) in the x-y plane perpendicular to the axis of symmetry at initial time t = 0. The surface plots of A and ϕ are also color coded by value. The red dashed lines below the surface mark the x coordinate of the center of the bubble. The circular lines below the surface trace the bubble rims.

2.3 Development of Numerical Methodology

1) A Novel Lyα Transfer Scheme on SPH: SEURAT

We have developed a novel Lyman alpha (Lyα) radiative transfer code, SEURAT (SPH scheme Extended with Ultraviolet line RAdiative Transfer), where line scatterings are solved adaptively with the resolution of the smoothed particle hydrodynamics (SPH) (Fig. 14). The radiative transfer method implemented in SEURAT is based on a Monte Carlo algorithm in which the scattering and absorption by dust are also incorporated. We perform standard test calculations to verify the validity of the code; (i) emergent spectra from a static uniform sphere, (ii) emergent spectra from an expanding uniform sphere, and (iii) escape fraction from a dusty slab. Thereby, we demonstrate that our code solves the Lyα radiative transfer with sufficient accuracy. We emphasize that SEURAT can treat the transfer of Lyα photons even in highly complex systems that have significantly inhomogeneous density fields. The high adaptivity of SEURAT is desirable to solve the propagation of Lyα photons in the interstellar medium of young star-forming galaxies like Lyα emitters (LAEs) (Abe et al. 2018).

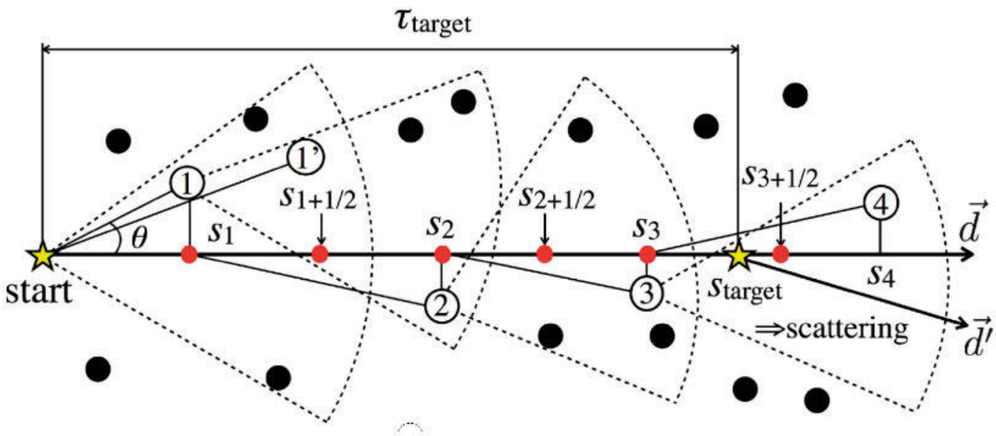

Figure 14: Schematic illustration of the ray-tracing scheme in SEURAT. The filled circles and numbered open circles represent the SPH particles. In the ray tracing, we search the downstream particle which is the closest to the ray. Grid points are determined by the projection of the downstream particles, as shown by red dots, and the optical depth is evaluated at intermediate points between two grid points. We do not use particle 1' as a downstream particle since particle 1 is closer to the ray, although particle 1' has the smaller angle. The dashed sectors represent the region where candidates for the next downstream particle are searched. Note that the radii of the sectors are not necessarily equal to the SPH smoothing length.

2) A New Scheme for General Relativistic Radiation Magnetohydrodynamics: UWABAMI

We develop a new scheme in which the full set of general relativistic radiation magnetohydrodynamic equations are solved on 3D spherical grids. In this scheme, the M1 closure approximation is employed. The frequency-integrated radiation fields are updated by solving the energy-momentum conservation equation for radiation. The free-free emission/absorption and Compton-scattering are included. The advective terms are explicitly solved by setting the simulation timestep based on the speed of light. On the other hand, the gas-radiation interaction terms (source terms) are implicitly solved because the timescale of the absorption/emission/scattering may be shorter than the light crossing time. To avoid singularities, we use Kerr-Shild metric.

3) A New Scheme for Multi-Frequency Radiative Transfer in Kerr Space-time: RAIKOU

We develop a new Monte Carlo radiation transfer code in which the multi-frequency radiation transfer equations are solved in Kerr space-time. Synchrotron emission/absorption, free-free emission/absorption, and Compton scattering are included. Especially, Compton cross section is correctly calculated by taking account of the electron temperature. The trajectory of the photon along the geodesic is calculated by the 8th-order Runge-Kutta method. This code can reproduce the photon-ring and was used in the analysis of the data of the Event Horizon Telescope.

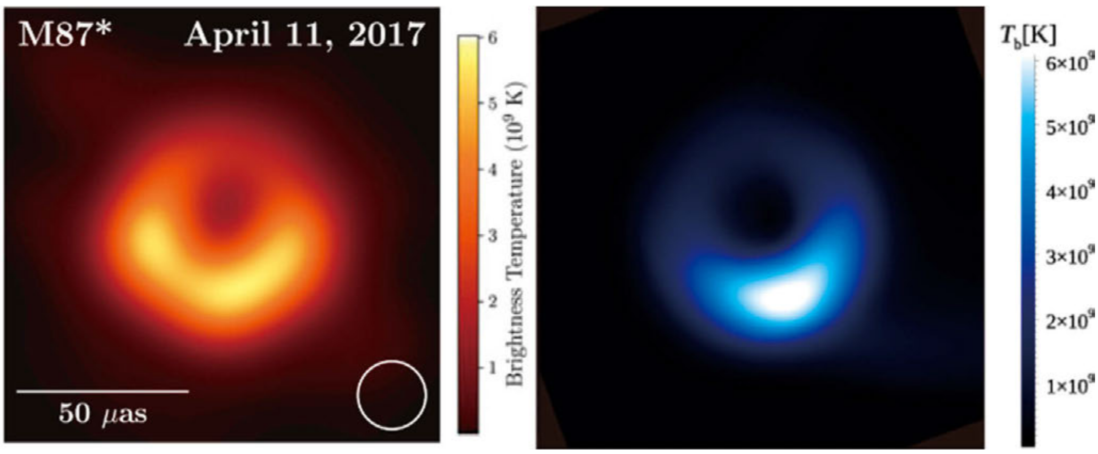

Figure 15: Photon-ring observed by Event Horizon Telescope (Left) and calculated by RAIKOU (Right). Resulting radio image obtained by RAIKOU is consistent with the observed image. In both images, the intensity of the bottom part of the ring is enhanced. This is expected to be due to the effect of the black hole spin, but the possibility of rotational motion of the gas cannot be ruled out.

4) General Relativistic Radiative Transfer Code in Rotating Black Hole Space-Time: ARTIST

As the first step to realizing the full general relativistic radiation hydrodynamics, we have developed a general relativistic radiative transfer code, ARTIST (Authentic Radiative Transfer In Space-Time), that is a perfectly causal scheme to pursue the propagation of radiation with absorption and scattering around a Kerr black hole (Takahashi & Umemura 2017). The code explicitly solves the invariant radiation intensity along null geodesics in the Kerr-Schild coordinates, and therefore properly includes light bending, Doppler boosting, frame dragging, and gravitational redshifts. The notable aspect of ARTIST is that it conserves the radiative energy with high accuracy, and is not subject to the numerical diffusion, since the transfer is solved on long characteristics along null geodesics. We first solve the wavefront propagation around a Kerr black hole that was originally explored by Hanni. This demonstrates repeated wavefront collisions, light bending, and causal propagation of radiation with the speed of light (Fig. 16). We show that the decay rate of the total energy of wavefronts near a black hole is determined solely by the black hole spin in late phases, in agreement with analytic expectations. We also explore the effects of absorption and scattering, and apply this code for a photon wall problem and an orbiting hotspot problem. All the simulations in this study are performed in the equatorial plane around a Kerr black hole.

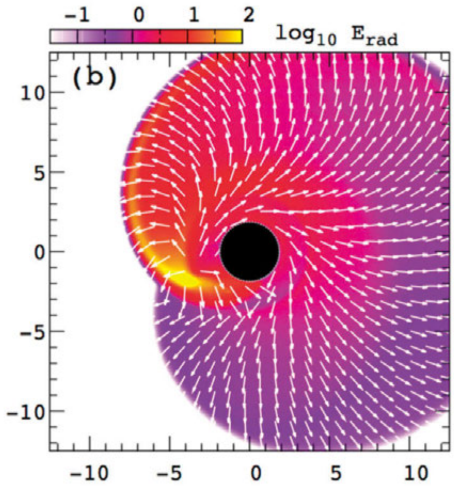

Figure 16: Snapshots of the radiation emitted from a hotspot orbiting a Kerr black hole. The radiation energy density is shown by color and the radiation flux vectors are shown by arrows.

5) GPU-accelerated Radiation Transfer/Hydrodynamic Simulation

We develop a new ray-tracing scheme to solve the transfer of diffuse radiation from spatially extended radiation sources on three-dimensional mesh grids that is efficient on processors with highly parallel architecture such as recently popular GPUs and CPUs with multi- and many-core architectures. We implement a new parallel radiation hydrodynamics code ‘ARGOT’, on the HA-PACS system (a GPU-equipped PC cluster installed at CCS) based on this scheme for the transfer of diffuse radiation. This code combines another scheme to solve radiation transfer from many point sources very efficiently by using the oct-tree structure for the distribution of radiation sources previously developed by our group. The performance of this code with the aid of GPUs to solve radiation transfer is higher than that without GPUs by nearly one order of magnitude.

Thus, it enables us, for the first time, to simultaneously compute the hydrodynamics and transfer of diffuse radiation such as recombination radiation of hydrogen, which is usually ignored in radiation hydrodynamic simulations of the structure formation in the early universe due to huge computational cost.

2.4 Collaborations

We have promoted and spread “Multidisciplinary Computational Sciences” with other research fields. One of them is “Computational Astrobiology (CAB)”, which is the collaboration between computational astrophysics, computational biology, and computational planetary science. In this collaboration, we have also pursued an active role in Exploratory Challenge on Post-K computer’ (Elucidation of the Birth of Exoplanets [Second Earth] and the Environmental Variations of Planets in the Solar System). Another collaboration is computational optical bioimaging in “Computational Medical Science (CMS)”, which is the collaboration among computational astrophysics, medical science, and mathematics. In addition, we have collaborated with High Performance Computing Systems division at CCS, for development of Cygnus and tuning of radiative transfer codes on Cygnus.

In the international collaborations, we have established the MOU with School of Physics and Astronomy, The University of Edinburgh, UK. Also, we have partnered with groups at Department of Physics and Astronomy, University of California at Los Angeles, Institute of Astronomy, University of Vienna, Mt Stromlo Observatory, Department of Physics and Astronomy, John Hopkins University, the Institut Astrophysique de Paris, and at the Observatoire de Paris, and with groups at Department of Physics and Astronomy, University of California at Los Angeles, Institute of Astronomy, University of Vienna, Department für Physik, Ludwig-Maximilians Universität München, Max Planck Institute for extraterrestrial Physics, Observatoire de la Côte d'Azur, Department of Physics & Astronomy, University of Waterloo.

1) Computational Astrobiology (CAB)

Recently, we have initiated “Organization for Computational Astrobiology”. Astrobiology has attracted a significant deal of attention owing to advanced observations of extrasolar planets as well as interstellar molecules. This organization aims at exploring key processes related to the origin of life in the universe through *ab initio* calculations based on collaboration among the Computational Astrophysics, Computational Biology, Computational Planetary Science, and Computer Science fields. These research efforts are targeted on the growth of dust grains in turbulent protoplanetary disks, the formation of interstellar molecules, and the generation of circularly-polarized light that could be responsible for the homochirality of amino acids.

■ Navier–Stokes Simulations on Dust Coagulation in a Turbulent Protoplanetary Disk

The coagulation of dust particles is a key process in planetesimal formation. However, the radial drift and bouncing barriers are not completely resolved, especially for silicate dust. Since the collision velocities of dust particles are regulated by turbulence in a protoplanetary disk, turbulent clustering should be properly treated. To that end, direct numerical simulations (DNSs) of the Navier–Stokes equations are requisite. We perform DNSs with up to Reynolds number Re=16,100, which allow us to track the motion of particles with Stokes numbers of 0.01≤St≤0.2 in the inertial range (Ishihara et al. 2018). Through the DNSs, we confirm that the rms relative velocity of particle pairs is smaller by more than a factor of two, compared to that by Ormel & Cuzzi (2007). The distributions of the radial relative velocities are highly non-Gaussian. We find that even in the strong-turbulence case with α-viscosity of 10^{-2}, the sticking rates are as high as ~50% and the bouncing probabilities are as low as ~10% (Fig. 17). Thus, turbulent clustering plays a significant role in the growth of centimeter-sized compact aggregates (pebbles) and also enhances the solid abundance, which may lead to the streaming instability in a disk.

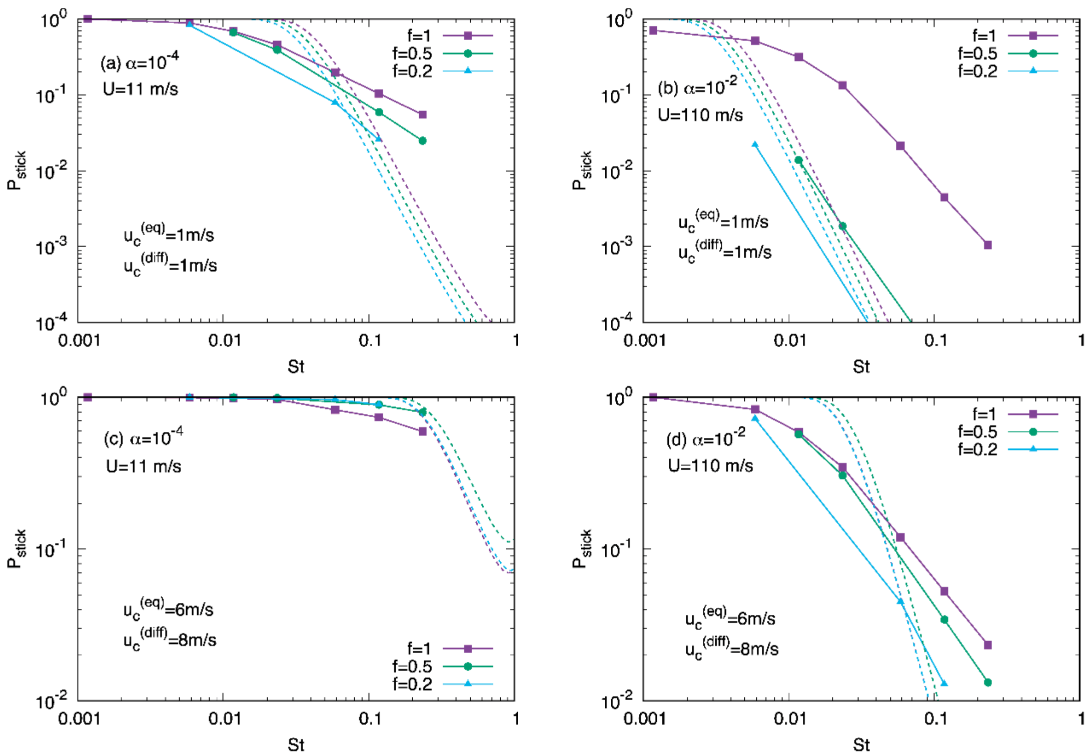

Figure 17: Sticking rates of colliding particles as a function of St, depending on f=St$_2$/St$_1$, for (a), (c) viscous parameter α=10^{-4} and (b), (d) α=10^{-2}. u_c is the critical collision velocity. Colored solid curves represent the DNS results. Colored dotted curves denote the theoretical prediction assuming a Gaussian (Maxwell) distribution whose variance is given by Ormel & Cuzzi (2007).

■ Formation of Glycine in Interstellar Environments

As a possible formation mechanism of glycine in astrophysical environments, a reaction path via aminoacetonitrile and hydantoin (2,4-imidazolidinedione), which have been detected in an interstellar cloud and meteorites, respectively, were analyzed using the density functional theory (Kayanuma et al. 2017). The formation of hydantoin from aminoacetonitrile via the Bücherer-Bergs reaction and the hydrolysis of hydantoin were investigated. The results showed that the catalytic water molecules significantly lower the reaction barriers for the formation of hydantoin. Although the highest barrier is still too high that the pathway is inactive in an interstellar medium, this reaction would proceed during the heating of the meteorite parent body.

■ Cosmic Origin of Homochirality of Amino Acids

After the discovery of the enantiomeric excess (ee) of amino acids in the Murchison meteorite, the cosmic origin of homochirality has been argued. The symmetry breaking of molecular chirality induced by circularly polarized light (CPL) is a possible solution. Recently, circularly polarized infrared emission has been observed in star-forming regions. However, the origin of CPL has not been revealed yet.

We study the generation of CPL induced by non-spherical dust grains in star-forming regions (Fukushima, Yajima, & Umemura, 2020, in preparation). Our Monte Carlo radiative transfer code follows changes of Stokes parameters in photon scattering. We argue that the observed high circular polarization (CP) (> 20%) can be explained by single scattering of the large dust grains as well as the dichroic extinction of scattered photons. In space, ionized hydrogen gas around star forming regions emits intense Lyman-α (Lyα) radiation, which could be responsible for ee of amino acids. We also explore the generation of circularly polarized Lyα radiation. As a result, we find that CP can be generated at a level of 10%-20% for grain sizes from 0.01μm-0.1μm (Fig. 18).

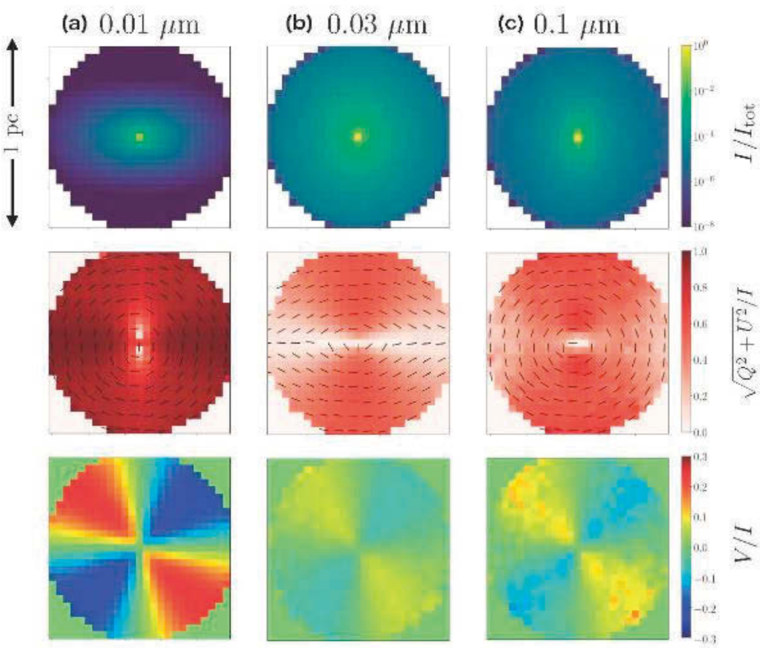

Figure 18: Monte Carlo simulation on the generation of circularly polarized Lyα radiation. Top panels show the intensity, middle panels linear polarization, and bottom panels circular polarization, respectively for grain size 0.01μm, 0.03μm, and 0.1μm.

2) Computational Optical Bioimaging

In recent years, the technology of optical imaging is extraordinarily developing, and thereby molecular processes in live cells and tissues can be pursued. The optical bioimaging can dynamically visualize multi-level function and morphological alteration in molecules and organs, and possesses a lot of advantages such as no exposure, non-invasion, bed side inspection, low cost, low restraint, and high time –resolution. Thus, it allows us to make automatic and remote diagnosis, monitoring, and screening and is applicable to new-born babies and infants without side effects like CT or MRI. Since biological tissues are strong scattering media, radiative transfer calculations are required to extract the local information from scattered light. In this project, we are developing a technology of CT with near-infrared imaging based on radiative transfer equation (Fig. 19).

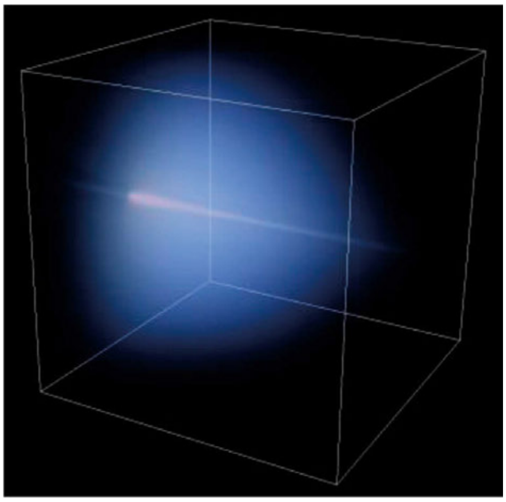

Figure 19: Radiative transfer calculation on the propagation of near-infrared light for a model of human body.

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2.6 Grants

1. Masayuki Umemura, JSPS Grant-in-Aid for Scientific Research (A), 2019-2023, 34,600,000 JPY
2. Alexander Y. Wagner, JSPS Grant-in-Aid for Scientific Research (C), 2019-2021, 2,600,000 JPY
3. Yuta Asahina, JSPS Grant-in-Aid for Young Scientists (B), 2018-2021, 2,600,000 JPY
4. Ken Ohsuga, JSPS Grant-in-Aid for Scientific Research (C), 2018-2020, 3,770,000 JPY
5. Hidenobu Yajima, JSPS Grant-in-Aid for Young Scientists (A), 2017-2020, 18200000 JPY
6. Hidenobu Yajima, JSPS Grant-in-Aid for Research Activity start-up, 2017-2020, 2730000

JPY

7. Kenji Furuya, JSPS Grant-in-Aid for Young Scientists (B), 2017-2020, 3,120,000 yen
8. Ken Ohsuga, JSPS Grant-in-Aid for Scientific Research on Innovative Areas, 2018-2019, 1,700,000 JPY
9. Hidenobu Yajima, JSPS Grant-in-Aid for Scientific Research on Innovative Areas, 2018-2019, 2600000 JPY
10. Kohji Yoshikawa, JSPS Grant-in-Aid for Scientific Research on Innovative Areas (JP18H04336), 2018-2019, 2,210,000 JPY
11. Kohji Yoshikawa, Priority Issue 9 on Post-K computer (Elucidation of the Fundamental Laws and Evolution of the Universe), 2015-2019, 33,371,000 JPY
12. Masayuki Umemura, JSPS Grant-in-Aid for Scientific Research (B), 2015-2018, 5,400,000 JPY
13. Masao Mori, JSPS Grant-in-Aid for Scientific Research (C), 2013-2018, 5,200,000JPY
14. Ken Ohsuga, JSPS Grant-in-Aid for Scientific Research (C), 2015-2017, 3,770,000 JPY
15. Ken Ohsuga, JSPS Grant-in-Aid for Young Scientists (B), 2012-2014, 2,730,000 JPY
16. Yuta Asahina, Grant-in-Aid for JSPS Fellows, 2012-2014, 2,700,000 JPY
17. Go Ogiya, Grant-in-Aid for JSPS Fellows, 2013-2014, 2,300,000 JPY

3 Division of Nuclear Physics

3.1 Overview

In the nuclear physics group, we perform theoretical and computational researches in nuclear many-body problems by developing new theories and computational methods for quantum many-body systems. Especially, our primary target is the theoretical investigation on nuclear structure, reaction, and neutron stars using energy density functional (EDF) method and its extension. In the following, we show major recent achievements since 2014, including nuclear reactions in the time-dependent approaches [section 3.2-1)], theories of large amplitude collective motion [section 3.2-2)], and structure of neutron stars [section 3.2-5)]. New theoretical approaches, such as the canonical-basis time-dependent Hartree-Fock-Bogoliubov theory and the finite amplitude method, which we have proposed before 2014, are further extended and adopted for studies of many kinds of nuclear phenomena [sections 3.2-1), 2)]. In addition, we propose new theories and computational methods, such as the requantization of time-dependent mean field [section 3.2-2)], the interacting boson model for odd nuclei [section 3.2-3)], and the Green's function for finite-temperature mean-field calculations [section 3.2-5)]. These developments are valuable not only in the basic science but also in various applications including nuclear engineering. In addition to the basic science, we also contribute to a program of transmutation of nuclear wastes [section 3.2-6)].

We utilize computational resources provided by several domestic institutes through the HPCI System Research Project (Project ID: hp140010, hp150081, hp160062, hp170068, hp170144, hp17081, hp180041, hp180066, hp180080, hp190031) and through Multidisciplinary Cooperative Research Program of CCS [section 5.5 in PART I].

3.2 Research Results

1) Time-dependent density-functional method for nuclear reaction of superfluid nuclei

We have developed theories and computer programs for time-dependent density functional theory (TDDFT) for nuclear systems with/without pairing correlations. Using those computer codes, microscopic reaction mechanisms, such as nuclear fusion and fission dynamics, have been studied and elucidated.

Effect of octupole deformation on the fission of actinides

One of our recent achievements is the description of nuclear fission in actinide nuclei that is a source of energy in nuclear reactors. Most of the actinide nuclei show asymmetric fission, in which, typically, the heavy fission fragments are Xenon and surrounding elements (with proton number $Z \approx 54$). The mechanism of this massive production of Xenon has been a longstanding puzzle. We use the canonical-basis time-dependent Hartree-Fock-Bogoliubov (Cb-TDHFB) theory [Ebata et al., Phys. Rev. C 82, 034306 (2010)] with Skyrme energy density functionals (EDFs) and find that heavy fragments are produced predominantly with 52 to 56 protons. This is associated with substantial octupole deformation of the heavy fragments acquired on the way to fission (Figure 1). These octupole shapes, which favor asymmetric fission, are induced by deformed shells at $Z = 52$ and $Z = 56$. Here, the spherical magic shell of $Z = 50$ turns out to be unfavored due to a strong resistance against the octupole deformation.

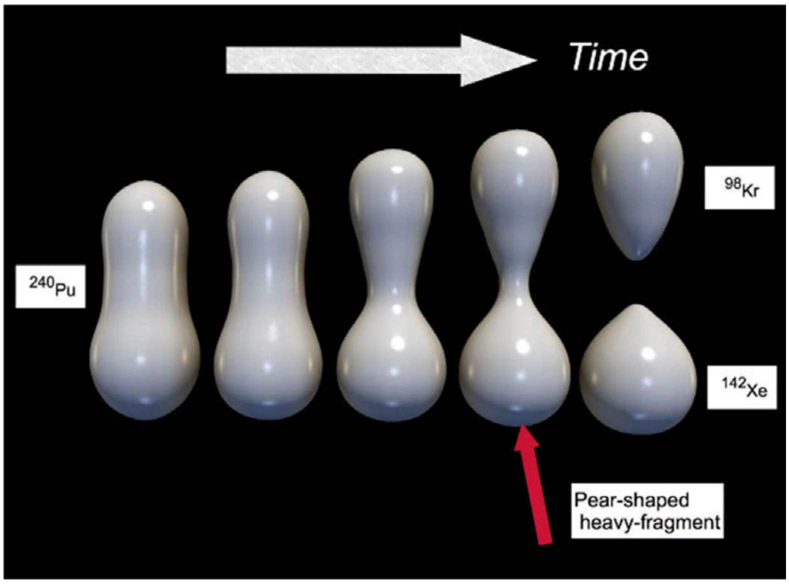

Figure 1: Shape evolution of fission of ^{240}Pu.

Dynamical pairing effect on nuclear reaction

The Cb-TDHFB is computationally feasible but an approximation of the full TDHFB theory. We have also developed a full TDHFB computer program with Gogny EDFs, and study dynamical pairing effects in the collision processes of superfluid nuclei. We perform simulations of colliding two superfluid nuclei, $^{20}O+^{20}O$. One of the characteristic features of superfluid systems is the presence of the gauge angle which is known to play a key role in the Josephson current. We find that the relative gauge angle between two nuclei affects the nucleus-nucleus potential and the fusion barrier height (Figure 2). An empirical study on the experimental fusion barriers shows a possible indication of the superfluidity. We also develop a new method of triple projection on the particle number, and find that the gauge angle also significantly affects the number of transferred neutrons. In order to study the nucleus-nucleus potential for superfluid nuclei, we propose an extension of the density-constrained TDHF (DC-TDHF) into the density-constrained TDHFB (DC-TDHFB) method. This method is applied to $^{20}O+^{20}O$ reaction, to quantify the effects of superfluidity on the nucleus-nucleus potential and on the fusion cross section.

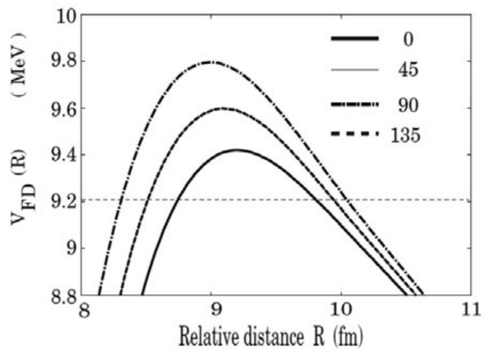

Figure 2: Potentials between two ^{20}O nuclei with different gauge angles.

Quasifission and superheavy element synthesis

Physics of superheavy elements (SHEs) is one of the most important topics in nuclear physics today. Since the SHE synthesis is strongly hindered by quasifission processes, it is important to understand its detailed mechanism. Using the TDDFT without pairing correlation, we perform a detailed analysis of quasifission processes in the $^{64}Ni+^{238}U$ reaction which may lead to the formation of the unknown element 120 (Figure 3). We find that the quasifission processes strongly depend on the quantum shells and orientations of deformed ^{238}U. From a comparison of the mass number and the total kinetic energy (TKE) of outgoing fragments with available experimental data, we demonstrate that the TDDFT is capable of quantitatively describing the main process of quasifission dynamics in collisions of heavy nuclei.

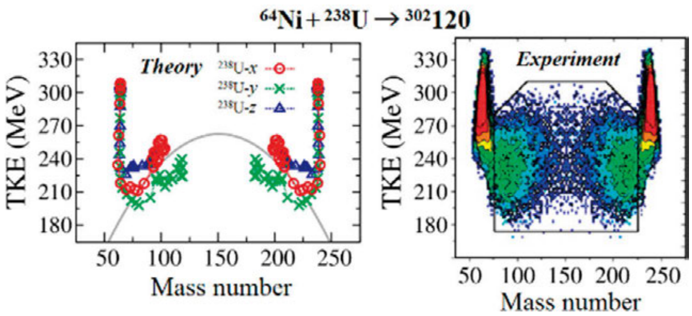

Figure 3: Calculated and experimental total kinetic energy (TKE) and mass number of fragments in $^{64}Ni+^{238}U$.

2) Nuclear collective motion and quantum large amplitude collective motion

Nuclei show many kinds of collective motion. At low energy, the nuclear collective dynamics exhibit strong quantum nature. For instance, nuclear shape fluctuation and shape coexistence phenomena are very important in transitional regions. Nuclear spontaneous fission and sub-barrier fusion reaction are typical examples of many-body quantum tunneling. These nuclear large amplitude dynamics at low energy cannot be studied by a naïve application of TDDFT, because of missing quantum effects in low-energy collective motions. In order to attack these difficult problems, we have been working on theories and methodologies of the large amplitude collective motion.

Developments in finite amplitude method and calculation of the Nambu-Goldstone modes

Linear response calculation such as quasiparticle random-phase approximation (QRPA) is a powerful tool to study nuclear collective modes of excitation. The conventional solution of the QRPA problem is based on the matrix diagonalization that needs additional model-space truncation for deformed calculation. An alternative approach we have been developing is the finite amplitude method (FAM), which formally provides a solution equivalent to the QRPA by the iterative procedure. Extension of the FAM formalism allows us to evaluate the QRPA sum rules, and zero-energy Nambu-Goldstone modes associated with the spontaneous symmetry breaking. Especially the analysis of the Nambu-Goldstone modes originated from the gauge symmetry breaking provides us with valuable information to construct sophisticated nuclear pairing EDF (Figure 4). We have also extended the FAM code developed based on the axial nuclear DFT solver HFBTHO for non-axial excitation, that allows us the full evaluation of the multipole modes such as photoabsorption cross section.

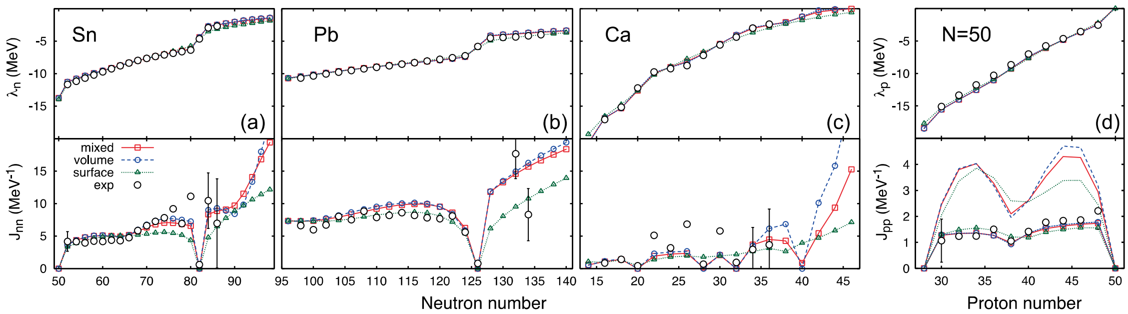

Figure 4: Chemical potentials (upper panels) and pairing rotational moments of inertia (lower) for neutrons in Sn, Pb, and Ca isotopes and for protons in $N = 50$ isotones.

Inertial masses for nuclear collective motion

In order to describe large-amplitude collective motion, a possible approach is to construct a collective Hamiltonian from the microscopic point of view. For instance, in nuclear structure calculations, the five-dimensional quadrupole collective Hamiltonian is well-known, for which we want to evaluate the collective inertial masses in the kinetic term, based on the nuclear EDF. To evaluate those inertial masses including dynamical residual correlation, we may utilize the QRPA method and the FAM to reduce its computational cost. The rotational moments of inertia in the collective space of the $\beta-\gamma$ plane for a transitional nucleus ^{108}Pd is shown as an example (Figure 5). The dynamical residual correlation, which is missing in the cranking (Inglis-Belyaev) formula, increases the rotational moments of inertia.

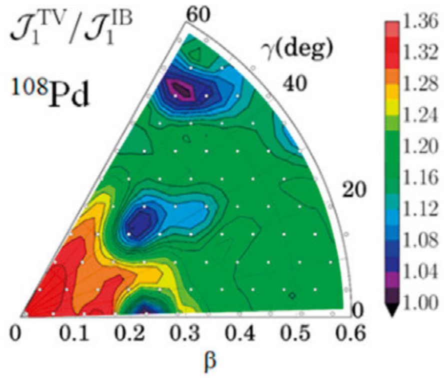

Figure 5: Ratio of rotational moment of inertia with and without dynamical residual correlations, J^{TV}/J^{IB}, for ^{108}Pd.

Reaction path and inertial masses for sub-barrier fusion

Using the adiabatic self-consistent collective coordinate (ASCC) method, we may self-consistently determine the optimal collective path, the collective potential, and the collective inertial masses. Then, we are able to construct the collective Hamiltonian for low-energy collective motion. Combining the imaginary-time method and the FAM, we achieve this goal for fusion reactions of light nuclei. We show here results for one of the alpha processes in which stars convert helium into heavy elements, $\alpha + {}^{16}O \rightarrow {}^{20}Ne$ (Figure 6). The calculated astrophysical S-factor indicates the importance of the self-consistent determination of the inertial masses for the fusion reaction.

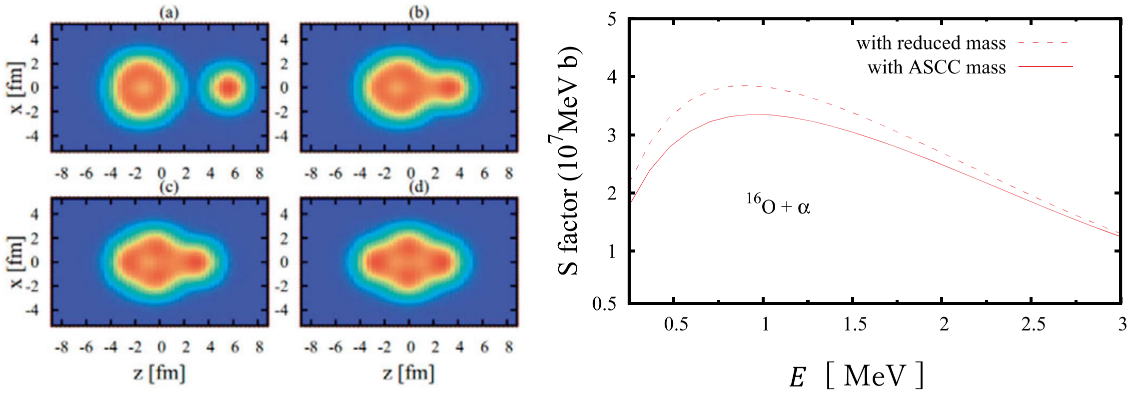

Figure 6: (Left panels) Density distribution on the ASCC fusion reaction path, $^{16}O+\alpha\rightarrow{}^{20}Ne$. (Right) Astrophysical S-factor calculated with the microscopically constructed collective Hamiltonian.

Novel way of constructing microscopic wave functions for collective motions

Instead of going through the collective Hamiltonian, it is also possible to directly construct microscopic wave functions representing nuclear collective motions. For integrable systems, a possible requantization method of the TDDFT has been known, according to the stationary phase approximation of the path integral formulation. However, it is not applicable to non-integrable systems in general. We propose a new approach of combining this with the ASCC method. The ASCC method is used to extract an integrable collective subspace which is approximately decoupled from the other intrinsic degrees of freedom. We apply the method to the pairing model and demonstrate its usefulness.

3) Interacting boson model with EDF method

We develop a theoretical method of describing spectroscopic properties of heavy nuclei, that is based on the frameworks of the nuclear EDF and the interacting boson model (IBM). Particularly, we work on its extension to odd-mass nuclear systems by using the particle-boson coupling scheme. In this method, the self-consistent EDF calculation provides microscopic inputs to the IBM calculations. The method allows for an accurate, systematic, and computationally feasible prediction of spectroscopy in heavy nuclei that are on the frontier of radioactive-ion-beam facilities. A number of applications were made, including microscopic calculations of the observables that signal the quantum/shape phase transitions in a number of odd-mass nuclei (Figure 7).

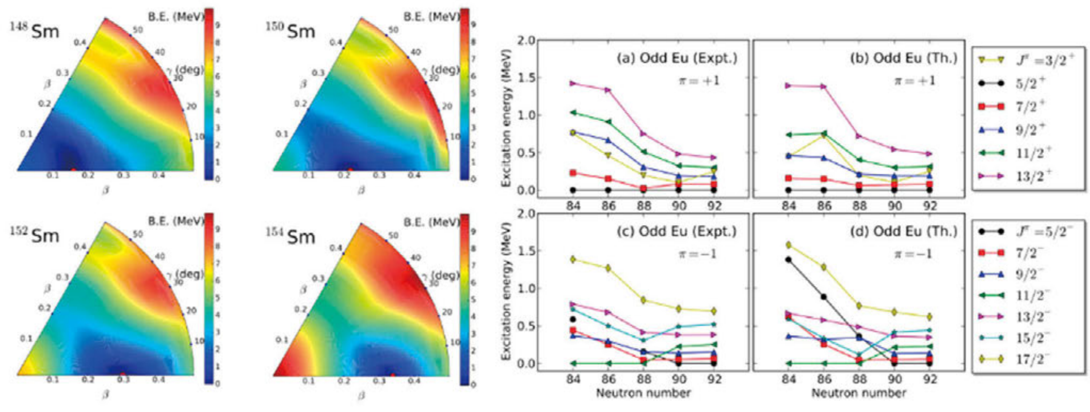

Figure 7: (Left) Potential energy surfaces in the (β,γ) plane for even-even $^{148\text{-}154}$Sm from the self-consistent EDF calculation. (Right) Low-lying spectra for the neighboring Eu isotopes.

4) Nuclear matrix element of neutrinoless double-beta decay

Neutrinoless double-beta decay has been investigated, as it will clarify the absolute value of the neutrino mass and mass hierarchy if the neutrino is a Majorana particle. The precise evaluation of the nuclear matrix element is required in order to derive the neutrino mass from the half-life. We perform a calculation based on the generator-coordinate method using the proton-neutron pairing amplitude as the generator coordinate, showing that the nuclear matrix element is suppressed by the isoscalar neutron-proton pairing. We also confirm that the suppression of the nuclear matrix element by the isoscalar pairing is also present in the shell model approach.

The role of the isoscalar neutron-proton pair is also studied by an isospin-invariant version of the IBM derived from a realistic shell-model Hamiltonian. The isoscalar pair in the model is important in the accurate prediction of the nuclear matrix elements for $N{\sim}Z$ nuclei in the mass $A{\sim}50$ region. The QRPA is another method for the nuclear matrix element, however, we need to evaluate the overlap between QRPA eigenstates built on parent and daughter nuclei. We find that this overlap substantially reduces the nuclear matrix element.

5) Structure of neutron stars and nuclear equation of state (EoS)

Neutron star EoS and dark matter

Recently, the gravitational waves from mergers of binary neutron stars were detected. The gravitational wave detection provides precious information on the neutron-star core equation of state (EoS). A single parameter, the tidal deformability, characterizes the dependence of the waveform of the gravitational radiation on the internal structure of neutron stars, allowing us to discriminate among different EoSs. We aim to develop accurate descriptions of nuclear matter and to relate nuclear microphysics to macroscopic observables.

Assuming relatively light Weakly Interacting Massive Particles (WIMP) as a dark matter candidate, realized in the Next-to-Minimal Supersymmetric Standard Model, the dark matter particle interacts with the baryonic matter through Higgs bosons. We use the effective field theory motivated relativistic mean field model to study the nuclear EoS in the presence of the dark matter. The calculated properties are compared with the corresponding data of the GW170817 event.

Finite-temperature Hartree-Fock-Bogoliubov calculation for inner crust

The inner crust of neutron stars plays an important role in various observed phenomena, such as cooling and pulsar glitches. The semi-classical approach, such as Thomas-Fermi theory and quantum molecular dynamics, predicts a variety of phases, called “pasta phase”, in the inner crust. To study these structures with the unrestricted EDF methods, we develop a Green’s function method for the finite-temperature Hartree-Fock-Bogoliubov (FT-HFB) calculation in the three-dimensional coordinate space. In this method, we do not have to diagonalize the HFB Hamiltonian, and it is suitable for massively parallel computing. Preliminary calculations suggest a possible new phase of pasta phase.

Vortex dynamics in the neutron star crust

One of the fascinating phenomena related to superfluidity and superconductivity, is "topological excitations" of superfluid, in the form of a quantized vortex. The vortex is also expected to play an important role in the inner crust of neutron stars. Especially, their pinning and unpinning on the nuclei are supposed to cause the pulsar glitch phenomena, namely, sudden change of rotational frequency of rotating neutron stars. Using a GP-GPU computer program for the full TDHFB with the Skyrme EDF, we find that a quantized vortex line of superfluid neutrons and a nucleus surprisingly repel each other, at least, at the neutron densities of $n_n = 0.014$ and 0.031 fm^{-3} (Figure 8). Moreover, we find the significance of internal degrees of freedom, "vortex bending" and "nuclear shape deformation". The results have an impact on the modeling and the interpretation of the pulsar glitch.

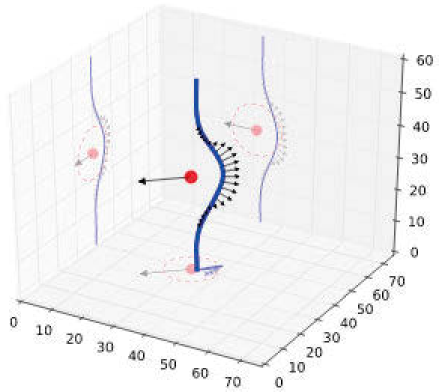

Figure 8: Vortex line and forces between a vortex and a nucleus.

6) Nuclear wastes and simulation of nuclear transmutation

The high-level radioactive wastes are planned to be disposed of through vitrification in glass solid and burial in deep geological layers. As these wastes contain nuclides with a long half-life, public concern remains over the long-term storage of such wastes. There is also a social problem in terms of the difficulty to determine disposal sites for these wastes. Since 2014, we participate in one of ImPACT programs, which aims at high-risk, high-impact R&D for a sustainable and expandable innovation system, "Reduction and Resource Recycling of High-level Radioactive Wastes through Nuclear Transmutation" (Figure 9). The goal of this program is to investigate the nuclear reaction paths for long lived fission products (LLFP). The establishment of reasonable nuclear transmutation methods will enable these wastes to be converted into stable nuclides or short-lived ones. Possibly, we may hope to develop ecological systems for the reuse of the rare metals and other resources that are included in the recovered products.

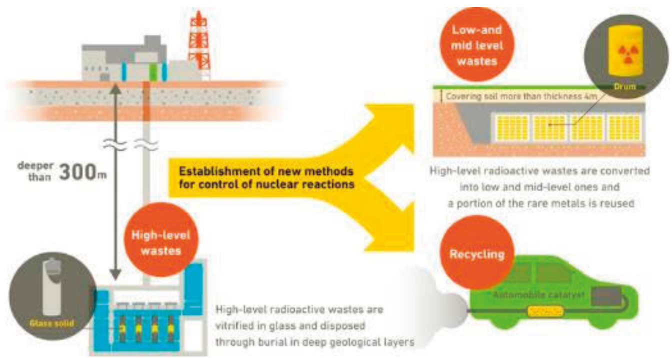

Figure 9: Basic concept of the program.

Nuclear structure data for simulation of nuclear transmutation

In the ImPACT program, we are in charge of constructing data of nuclear structure properties necessary for the calculation of reaction cross sections. Using the Skyrme EDF approaches with the three-dimensional coordinate-space representation, we systematically calculate ground-state properties, single-particle energies and wave functions, photoabsorption cross sections, neutron capture cross sections, etc. Then, these data are provided as basic inputs for a simulation code PHITS (Particle and Heavy Ion Transport code System) of nuclear transmutation for bulk systems. The importance of secondary neutrons is suggested by the simulation (Figure 10).

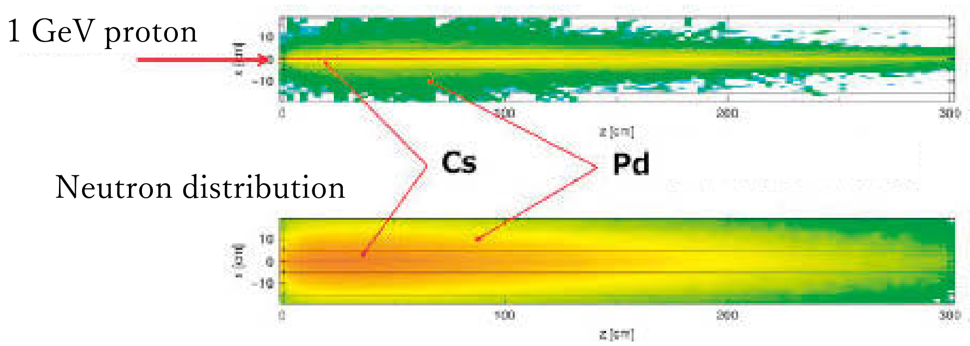

Figure 10: PHITS simulation of transmutation of ^{107}Pd and ^{135}Cs by injected protons at 1 GeV.

Computational nuclear data and InPACS

The simulation of the nuclear transmutation requires reaction data of many nuclides, because their reaction paths are not unique. We perform the unrestricted EDF calculation with the three-dimensional coordinate-space representation for all the nuclides up to the actinide region. In order to provide these data for future applications of many kinds, we open a web site, InPACS (Interactive Plot of Atomic nuclei and Computed Shapes, Figure 11), and show the calculated ground-state deformation, binding energy, density distribution, neutron/proton separation energy, etc. Furthermore, we provide tutorial Q&A for the public about nuclear physics and nuclear transmutation.

InPACS
Interacting Plot of Atomic nuclei & Computed Shapes

Figure 11: InPACS logo and its QR code.

3.3 Collaboration

Regular collaborative meetings on nuclear EDF approaches and computational methods among several domestic institutes are held roughly every month, and our institute plays a central role in this collaboration. Major institutes participating in this activity are RIKEN, the University of

Tokyo, Niigata University, and Kyoto University. A number of theory-theory and theory-experiment collaborations have been engaged since 2014. We have been collaborating with many foreign researchers, especially, those in Warsaw University of Technology for developments of GP-GPU program of TDDFT [sections 3.2-1) and 5)], Michigan State University and University of Jyväskylä for FAM code with HFBTHO [sections 3.2-2) and 5)], University of Zagreb for IBM studies [section 3.2-3)], and Australian National University for fusion/fission studies [section 3.2-1)]. A member of our group (T.N.) has been the principal investigator for JSPS international collaboration programs, the bilateral programs [Japan-US (2014), Japan-China (2017-2019)] as the principal investigator, and the investigator for A3 foresight program [Japan-China-Korea (2019-2024)]. N.H. has been participating in a US SciDAC-3 project "NUCLEI" (2012-2017) as a foreign collaborator.

3.4 Future Plan

We plan to study nuclear collective motion, nuclear reaction, and physics of neutron stars, developing novel theories and efficient computational methodologies. One of main topics in near future is a microscopic theory of nuclear reaction at low energy, discussed in Sec. 3.2-2). We would like to apply the method to heavier systems and include the pairing correlations. The structure of neutron stars is another topic we would like to further investigate (Sec. 3.2-5)). Especially, we plan to study structure of the inner crust and properties of free neutrons. These properties are indirectly observed, for instance, as pulsar glitch phenomena.

3.5 Publications

Journal Papers (refereed)

1. K. Wen and T. Nakatsukasa, Collective inertial masses in nuclear reactions, accepted by Front. Phys. [Invited paper]
2. J. Ha, T. Sumikama, F. Browne, N. Hinohara, A. M. Bruce, S. Choi, I. Nishizuka, S. Nishimura, P. Doornenbal, G. Lorusso, P.-A. Soderstrom, H. Watanabe, R. Daido, Z. Patel, S. Rice, L. Sinclair, J. Wu, Z. Y. Xu, A. Yagi, H. Baba, N. Chiga, R. Carroll, F. Didierjean, Y. Fang, N. Fukuda, G. Gey, E. Ideguchi, N. Inabe, T. Isobe, D. Kameda, I. Kojouharov, N. Kurz, T. Kubo, S. Lalkovski, Z. Li, R. Lozeva, H. Nishibata, A. Odahara, Zs. Podolyak, P. H. Regan, O. J. Roberts, H. Sakurai, H. Schaffner, G. S. Simpson, H. Suzuki, H. Takeda, M. Tanaka, J. Taprogge, V. Werner, and O. Wieland, Shape evolution of neutron-rich ^{106,108,110}Mo isotopes in the triaxial degree of freedom, accepted by Phys. Rev. C

3. N. Hinohara, Energy-weighted sum rule for nuclear density functional theory, Phys. Rev. C 100, 024310 (2019)
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2. 中務孝、他多数、「放射科学の事典」（朝倉書店、2015）[in Japanese]

Awards

Kai Wen, ANPhA/AAPPS-DNP award for young scientist, issued by Asian Nuclear Physics Association and Association of Asia Pacific Physical Societies Division of Plasma Physics, at the 18th CNS International Summer School. Aug. 27th, 2019.

Young Scientist Award of the Physical Society of Japan are awarded to the following former students who obtained PhD in our group.

- Kazuyuki Sekizawa, Awarded 2016.03 (PhD, March 2015)
- Shuichiro Ebata, Awarded 2015.03 (PhD, March 2011)

3.6 Grants

1. T. Nakatsukasa, JSPS Grant-in-Aid for Scientific Research on Innovative Areas (Research in a Proposed Research Area), 2019-2020, 2,630,000 yen
2. T. Nakatsukasa, JSPS Grant-in-Aid for Scientific Research(B), 2018-2021, 17,160,000 yen
3. N. Hinohara, JSPS Grant-in-Aid for Scientific Research on Innovative Areas (Research in a Proposed Research Area), 2017-2018, 2,600,000 yen
4. N. Hinohara, JSPS Grant-in-Aid for Young Scientists(B), 2016-2019, 3,770,000 yen
5. T. Nakatsukasa, JSPS Bilateral Joint Research Project (Japan-China), 2016-2018, 4,312,500 yen
6. K. Nomura, JSPS Grant-in-Aid for JSPS fellows, 2016-2017, 2,990,000 yen
7. T. Nakatsukasa, JST ImPACT Fujita program, “Reduction and Resource Recycling of High-level Radioactive Wastes through Nuclear Transmutation”, 2014-2018, 27,922,000 yen
8. J. Terasaki, JSPS Grant-in-Aid for Scientific Research on Innovative Areas (Research in a Proposed Research), 2015-2016, 2,340,000 yen.
9. J. Terasaki, JSPS Grant-in-Aid for Scientific Research(C), 2014-2016, 4,680,000 yen.
10. T. Nakatsukasa, JSPS Bilateral Joint Research Seminar (Japan-US), 2014, 2,484,000 yen
11. T. Nakatsukasa, JSPS Grant-in-Aid for Scientific Research(B), 2013-2016, 18,850,000 yen

4 Division of Quantum Condensed Matter Physics

4.1 Overview

Among diverse subjects in condensed matter physics, we focus our research activities on a few characteristic directions. In code developments, we have been developing our own computer codes based on density functional theory using a real-space grid representation. In scientific aspects, our activities primarily focus on light-matter interactions in various systems/occasions.

As for the code development, Yabana and his collaborators have been developing a computer code SALMON under close collaboration with Prof. Taisuke Boku's group in the Division of High Performance Computing Systems. The core part of the SALMON is a calculation of electron dynamics in real-time based on first-principles time-dependent density functional theory (TDDFT). Ono, who recently left our division, and his collaborators have been developing a computer code RSPACE that is based on first-principles density functional theory utilizing real-space finite-difference scheme. RSPACE is focusing first-principles calculations of transport phenomena in junctions and interfaces.

As for scientific aspects, Yabana has been applying SALMON to various phenomena induced by ultrashort laser pulses and produced fruitful results in attosecond science under close collaborations with experimental groups. Sato, who recently joined our division as an International Tenure-Truck Professor, has also been actively working on ultrafast dynamics in crystalline solids. Tong has been actively working in the field of AMO, atoms, molecules, and optics. He develops his own computer code solving time-dependent Schrödinger equation accurately in 2D and 3D geometries and has been collaborating with world-wide experimental groups on forefront ultrafast phenomena in atoms and molecules. Maeshima has been working on light-matter interactions in solids and nano-sized systems utilizing modeled Hamiltonian such as Hubbard model for strongly-correlated electronic systems, polaronic-quasiparticle model for optical phonon generation, and Floquet theory for semiconductor superlattice systems.

Besides researches on light-matter interaction, Ono has been working on transport phenomena at interfaces aiming at establishing the computational formalism to design the future electronics materials and devices. He has investigated electronic and atomic structures of SiC MOS structure and calculated carrier scattering property. Koizumi has been working on elucidating the mechanism of the high temperature superconductivity in cuprates. He and collaborators have developed a theory that utilizes the Berry connection for many-many body wave functions where the supercurrent generation is explained as a consequence of the existence of non-trivial Berry connection. He is also working on the theoretical study for the realization of the quantum computer using the cuprate as qubits.

4.2 Research Results

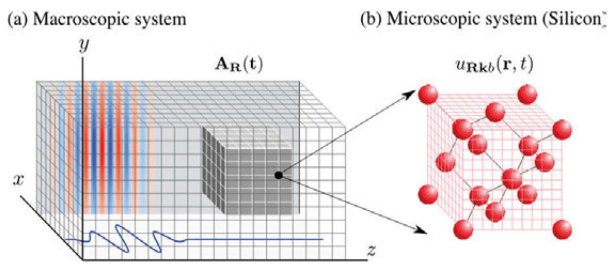
1) Development of first-principles electron dynamics simulation code SALMON

Yabana and his collaborators have been developing an open-source computer code SALMON (**S**calable **A**b-initio **L**ight-**M**atter simulator for **O**ptics and **N**anoscience). SALMON is capable of calculating electron dynamics and optical properties of molecules, nanostructures, and crystalline solids based on first-principles TDDFT. It can also carry out electromagnetism analysis using finite-difference time-domain method. As a unique feature of the code, SALMON is capable of carrying out light propagation simulation via coupling the electron dynamics in many microscopic unit cells using Maxwell's equations describing the time evolution of the electromagnetic fields. The code is efficiently parallelized so that it may describe the electron dynamics in large systems including up to a few thousand atoms. At present, we are making efforts of performance tuning of the code so that it runs efficiently at the new supercomputer FUGAKU in Japan under a close collaboration with the group of Prof. Boku. The code is open-source, freely downloadable at http://salmon-tddft.jp. The development of SALMON has been financially supported by several grants including CREST project in the strategic objective of Advanced Photonics organized by JST, Japan, and a project of a priority issue theme 7 to be tackled by using Post-K Computer organized by MEXT, Japan.

2) Ultrafast dynamics in solids under strong laser field

Yabana and his collaborators have been developing theoretical and computational methods to describe light-matter interactions in solids and nano-materials based on first-principles time-dependent density functional theory for more than 20 years. The methods are implemented in the open-source code SALMON, as mentioned above. Sato has been collaborating with the project, earlier as a PhD student and now as a staff member. Among various phenomena in optical sciences, applications to interactions of attosecond pulses with solids have been shown remarkable successes. We have carried out intimate collaborations with attosecond experimental groups including Max-Planck Institute for Quantum Optics, Germany, and ETH Zürich, Switzerland. For example, modulations of optical properties of dielectrics within a period of optical pulses have been measured using attosecond pulses, and our numerical calculations solving Maxwell and time-dependent Kohn-Sham (TDKS) equations simultaneously (Fig. 1 (Left)) have been successful to reproduce experimental measurements and to interpret the mechanism, as shown in Fig. 1 (Right). It has also been successful to explore nonlinear energy transfer mechanism from a visible pulsed light to electrons in a wide bandgap material.

We further extend our research in various directions: We consider a coupling with the lattice dynamics using Ehrenfest molecular dynamics solving the Maxwell, the TDKS, and the Newton equations simultaneously. It has been used to describe a generation of coherent phonons and a birth and amplification of Raman waves. We have also developed a novel and unified scheme to describe the interaction of ultrashort light pulses with two-dimensional materials, from atomic monolayers to thick films. We also develop a quantum-mechanical scheme to describe meta-surface, a two-dimensional sheet material composed of nano-particles.



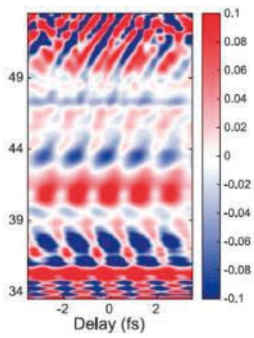


Figure 1 (Left) Grid system used in multi-scale Maxwell-TDDFT calculations. (Right) Modulation of optical absorption of probe pulse in diamond during irradiation of an intense and ultrashort pulse.

3) Time-dependent Schrödinger equation approach for ultrafast dynamics in atoms and molecules

In the past six years, Tong had mainly worked on the ultrafast dynamics of atoms and molecules in strong laser fields. By numerical simulation and collaboration with other research groups worldwide, (1) we explained the Coulomb effect on the photoionization of atoms in strong linearly as well as elliptically polarized laser fields; (2) investigated the frustrated tunneling ionization on the atomic excitation in a strong elliptically polarized laser field; (3) understood the mechanism of the moderate intense IR laser assisted XUV photoionization and photodissociation of molecules and found a way to control the dynamic processes by tuning the time-delay between the two pulses in an attosecond time scale; (4) calibrated the strong IR laser intensity at 1% level; (5) provided a way to measure the atomic energy structures by attosecond quantum beat. We also unveiled the mechanism of the dominance of the Breit interaction in dielectronic recombination of electron with highly charged ions and explored the electron-electron correlation effect on the antiproton-atom collision process. Meanwhile, we have also developed a new time-dependent density function theory method based on the fast Fourier transform for isolated many-atom systems in ultrashort intense laser fields.

To cope with the current research interests of the laser material interaction and his near future plan, he shows one of his works on the justification of applying the norm-conserving pseudopotential to laser-matter interactions. Norm-conserving pseudopotential is widely used in condensed matter physics for structure simulation since it circumvents the Coulomb singularity. For dynamic processes, like intense laser matter interaction, it has been used without justification. Or more specifically, without knowing the validity region. In this work, He and his collaborators compared the TDDFT simulations with an all-electron and with norm-conserving pseudopotentials to justify the application of norm-conserving pseudopotentials. There are two major processes in intense laser matter interactions. One is high-order-harmonic generation (HHG) and the other is above-threshold ionization (ATI). By the comparison, we found that pseudopotentials are reliable for the ATI over a broad range of laser intensity as shown in Fig. 2 (left), while they are applicable for low-order HHG as shown in Fig. 2 (right).

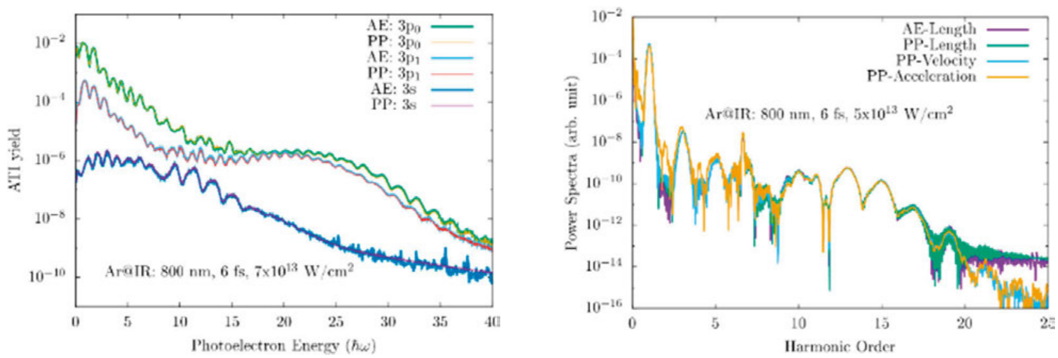


Figure 2 Ionization probabilities (left) and HHG yields (right) of Ar atoms in intense laser fields calculated with all electron potential and normal conserving

4) Photoinduced dynamics in electronic model systems

Maeshima has been studying the physical properties of a photoexcited state of a two-orbital Hubbard model at quarter filling on a 2 × 2 × 2 tetragonal cluster. Numerical analysis by using the Lanczos diagonalization method demonstrates that the dominant spin correlation drastically changes upon photoexcitation from the C-type antiferro (AF) correlation of the ground state to the A-type AF correlation of the photoexcited state.

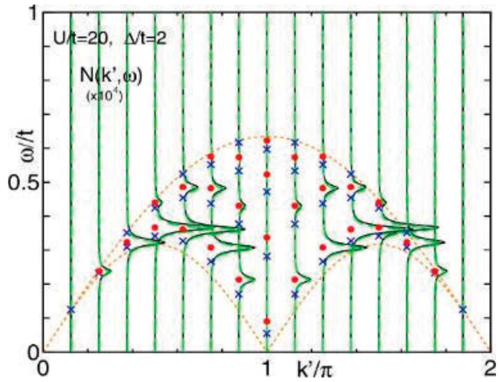


Figure 3 Charge dynamical structure factors N(k,ω) of the 1D ionic Hubbard model(green dashed lines) and that of the corresponding Heisenberg model (black solid

In addition, we investigate the charge dynamical structure factor N(k,ω) of a one-dimensional (1D) ionic Hubbard model in the Mott insulator (MI) phase. We show that the low-energy spectrum of N(k,ω) is expressed in terms of the spin operators for the spin degrees of freedom. The numerical results for the spin degrees of freedom well reproduce the low-energy spectrum of N(k,ω) of the 1D ionic Hubbard model, as shown in Figure 3.

In addition, we examine generation dynamics of coherent phonons in bulk semiconductors based on a polaronic-quasiparticle (PQ) model, where the PQ operator is composed of a quasiboson operator and a longitudinal optical (LO) phonon operator. By using this PQ model, we numerically calculate the photoemission spectra of semiconductors, and the obtained results show that in undoped Si, an asymmetric spectral profile characteristic of Fano resonance comes into existence immediately after the instantaneous carrier excitation to fade out gradually, whereas in undoped GaAs, no asymmetry in spectra appears in the whole temporal region. These results are in harmony with the reported experimental results.

We also study a resonance structure of Floquet state in dynamic fractional Stark ladder realized in biased semiconductor superlattices driven by a terahertz CW laser on the basis of the R-matrix Floquet theory. We calculate an excess density of state corresponding to the lifetime of the Floquet state with a fractional matching ratio η, where η is the ratio of a Bloch frequency to a laser frequency. Obtained results demonstrate the appearance of discernibly large peaks associated with Floquet states with longevity in a region of relatively high laser-intensity.

5) Development of first-principles electronic structure and transport property calculation code RSPACE

Ono has developed the first-principles calculation code, RSPACE, based on real-space finite-difference method. RSPACE enables us to calculate electronic structure and transport property of nanostructures. In the transport calculation, the computation of the self-energy matrices of electrodes, which are constructed from generalized Bloch waves, is time consuming. By exploiting the sparseness of the coefficient matrices of the real-space finite-difference method and using the Sakurai-Sugiura projection method, we efficiently solve the derived eigenvalue problem for the propagating and slowly decaying/growing evanescent waves, which are essential for describing the physics of surface/interface states and succeed to reduce computational cost for obtaining the self-energy matrices. By using full nodes of Oakforest-PACS, we have calculated the transport property of BN doped carbon nanotube consisting of more than 30,000 atoms and revealed that the characteristic behavior in the conductance spectrum, which appears in the small carbon nanotube, disappears.

6) Investigation of carrier scattering property of SiC-MOS

SiC has attracted considerable attention owing to its excellent physical properties, such as its high thermal conductivity, high breakdown strength, and large band gap. However, unlike Si MOS, SiC MOS has unacceptably low carrier mobility. One of the origins of the low carrier mobility is the generation of a large number of interface defects at the SiC/SiO2 interface. Ono reported that the carrier mobility increases when the interface defect density is reduced. To increase the carrier mobility of SiC MOS, understanding and precise control of the electronic structure of the SiC/SiO2 interface are indispensable. We have investigated the effect of oxidation of SiC by RSPACE and found that the oxygen insertion between Si and C causes carrier scattering. Since the oxygen insertion does not cause carrier scattering in Si MOS, our finding for characteristic scattering mechanism in SiC MOS gives experimentalists the guidelines to suppress carrier scattering in SiC.

7) Strongly-correlated systems

Koizumi and his collaborators have developed a method to calculate the Berry connection and current produced by it in a model for the cuprate superconductors. In this model, the conduction electrons perform spin-twisting itinerant motion and form spin-vortices. Then, a non-trivial Berry connection arises, and the spin-vortex-induced loop current (SVILC) is generated. In this model, a macroscopic supercurrent is generated as a collection of the SVICs.

It is known that the superconducting transition temperature Tc of the cuprate is not the energy gap formation temperature, but corresponds to the stabilization temperature of the superconducting coherence length sized loop currents. The SVILC corresponds to this loop current. Koizumi et al. have shown by performing the Monte Carlo simulation that indeed the

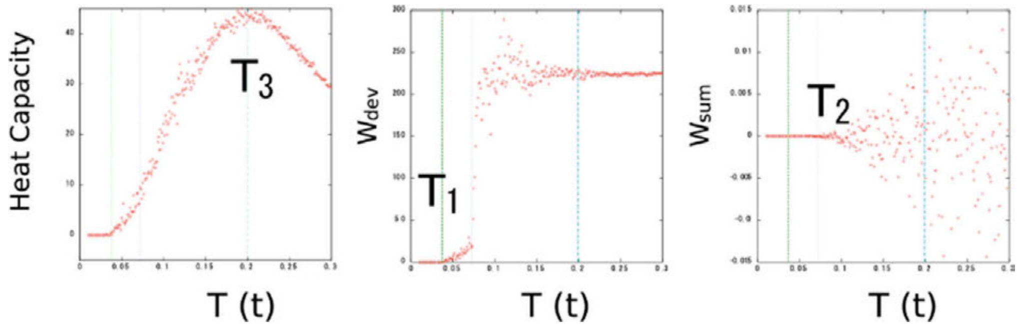


Figure 4 The Monte Carlo simulation for the SVILC model of the cuprate. There are three characteristic temperatures. T_1: the temperature above which the winding numbers for SVLCs start to change, corresponding to T_c. T_2: the temperature above which the total winding numbers for SVLCs start to change, may corresponding to the pseudogap temperature. T_3 : the temperature where the heat capacity has a maximum.

stabilization temperature of the SVILCs gives Tc values for the optimally doped sample.

As a by-product of the supercurrent generation by the Berry connection, a solution is given to a long-standing puzzling problem that the 'flux rule' (the Faraday's induction formula) contains two physics; one is the Lorentz force based emf, and the other is one of Maxwell's equations. It was found that the duality that a U (1) phase factor added on a wave function describes a whole system motion and also plays the role of a U(1) gauge potential leads to the same 'flux rule' for the classically two physics. This work is further enlarged by showing that superfluidity phenomena in general, including those found in boson systems can be also explained by the corrective mode arising from the Berry connection for many-body wave functions. As to the research on using SVILCs as qubits, we have performed the simulation of the Glover's algorithm. We have also obtained the patent license for using SVILCs as qubits in Japan and the USA. We expect that quantum computers with operation temperature at the liquid nitrogen temperature can be constructed using the cuprate and SVILCs.

4.3 Collaboration

1) Inside Center

Yabana has been collaborating with Prof. Boku's group of Division of High Performance Computing Systems on the code development and performance tuning of SALMON. He also joins meetings of Division of Nuclear Physics regularly where he is co-affiliated.

2) Collaboration in Japan

Yabana has been collaborating with Dr. Tomohito Otobe, Kansai Photon Science Institute on the code development of SALMON, and with Prof. Kenji Iida, Hokkaido University, and Prof. Takashi Yatsui, the University of Tokyo, on near-field optics.

Sato started a new collaboration with Prof. Kanemitsu's group of Kyoto University in the joint theory-experiment project on high-order harmonic generation from two-dimensional materials.

Tong has been collaborating with Prof. N. Nakamura's group of the University of Electro-Communications on investigating the collision processes in Tokyo Electron Beam Ion Traps.

Maeshima has been collaborating with Prof. M. Hase's group in University of Tsukuba on investigating laser-induced coherent phonon generation in semiconductors.

Ono has been collaborating with Dr. Yoshiyuki Egami of Hokkaido University on developing the RSPACE code and also collaborating with experimental group members of Osaka University, National Institute of Advanced Industrial Science and Technology, and University of Tsukuba on investigation of carrier mobility of SiC MOS.

Koizumi made a collaboration with Prof. M. Tachiki in Tohoku University on the cuprate problem and some other superconductivity related problems.

3) International Collaborations

Yabana has been collaborating with a group of Prof. J. Burgdörfer of Vienna University of Technology on theoretical TDDFT calculation. He has also been collaborating with the experimental group led by Prof. M. Schultze of Graz University of Technology and attosecond experimental group at Max Planck Institute for Quantum Optics. He recently joined a collaboration in the framework of Horizon2020-MSCA-RISE "Atlantic" project that is aiming to establish an international research network and collaborations on simulations of laser-matter interaction. He is also starting collaborations with Dr. M. Kozak, Charles University, Czech Republic, Prof. Guillaume Duchateau, Univ. of Bordeaux, France, and Prof. O. Uteza, Univ. Marseille, France.

Sato is in the position of International Tenure-Truck Assistant Professor, and stays at Max-Planck Institute for Structure and Dynamics of Matter, Hamburg, Germany, as his base of activity. There he is collaborating with. Prof. A. Rubio on light-induced nonequilibrium electron dynamics in matter. He is also collaborating with Prof. U. Kellter of ETH Zürich, and Prof. M. Nisoli and Dr. M. Lucchini of Politecnico di Milano on joint theory-experiment research for attosecond electron dynamics in solids. He is collaborating with Prof. A. Castro of University of Zaragoza on photo-induced nonequilibrium molecular dynamics, and Dr. A. Kelly of Dalhousie University on theory development for nonequilibrium electron-ion mixed systems.

Tong has been developing international collaborations with several institutes worldwide, Vienna University of Technology, Prof. J. Burgdörfer's group (theory): on many dynamic processes of atoms, molecules in an intense laser field as well as antiproton collision with atoms, University of Colorado Boulder, Profs. H. Kapteyn & M Murnane’s group (experiment): on atomic ionization in two-color circularly polarized laser fields and molecular dissociation processes in combined XUV and IR laser fields, and Griffith University, Centre for Quantum Dynamics Profs. R. Sang and I. Litvinyuk’s group (experiment): on frustrated tunneling ionization for atomic excitation in ultrashort laser fields and attosecond streaking for molecules in elliptically polarized laser fields.

Ono has been developing international collaborations with group members of Prof. S. Bluegel of Forcshungszentrum Juelich on developing the new computational methods and RSPACE code.

Koizumi made a collaboration with Prof. M. Abou Ghantous in Texas A & M University on the cuprate problem.

4.4 Future Plan

In computational optical science, we continue to develop the open-source code SALMON. As an urgent issue, we will carry out performance tuning so that it runs efficiently at FUGAKU, a new supercomputer in Japan. The goal in the future will be to make SALMON as one of the de-facto standard codes in the field of computational nano-optics. We expect to develop our computational approach and apply it to forefront research frontiers related to various light-matter interactions. We also expect to extend the theoretical modeling for light-induced electron dynamics in solids in order to unlock optical-control of material functionalities.

In the field of atoms, molecules, and optics, we will extend our present numerical methods for more general dynamic processes of matter intense laser interactions to collaborate with ongoing experiments. We will also continue our works on ion-atom collision.

In the field of strongly correlated systems, we improve the way to calculate electronic states that involve non-trivial Berry connection. This will lead to the elucidation of the mechanism of the cuprate superconductivity and enlarge our knowledge on the appearance of supercurrent.

We will consider architectures for quantum computers using SVILCs qubits, including the qubit design and killer applications for quantum computers.

4.5 Publications

Journal Papers (refereed)

1. N. Tancogne-Dejean, M. J. T. Oliveira, X. Andrade, H. Appel, C.H. Borca, G. Le Breton, F. Buchholz, A. Castro, S. Corni, A.A. Correa, U. De Giovannini, A. Delgado, F.G. Eich, J. Flick, G. Gil, A. Gomez, N. Helbig, H. Hübener, R. Jestädt, J. Jornet-Somoza, A. H. Larsen,

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2. D. Manabe and H. Koizumi, "Explanation of superfluidity using the Berry connection for many-body wave functions", J. Supercond. Nov. Magn. https://doi.org/10.1007/s10948-020-05438-w (2020)
3. M. Lucchini, S.A. Sato, F. Schlaepfer, K. Yabana, L. Gallmann, A. Rubio, U. Keller, "Attosecond timing of the dynamical Franz-Keldysh effect", Journal of Physics: Photonics, 2, 025001 (2020).
4. A. Hashmi, K. Nakanishi, T. Ono, "Graphene-based symmetric and non-symmetric magnetoresistive junctions", J. Phys. Soc. Jpn. 89, 034708 (2020).
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11. A. Yamada and K. Yabana, "Energy transfer from intense laser pulse to dielectrics in time-dependent density functional theory", Euro. Phys. J. D**73**, 87 (2019).
12. A. Yamada and K. Yabana, "Multiscale time-dependent density functional theory for a unified description of ultrafast dynamics: Pulsed light, electron, and lattice motions in crystalline solids", Phys. Rev. B**99**, 245103 (2019).
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Awards

Sato received a Young Scientist Award of the Physical Society of Japan, 2020, in division 5 (Optical Properties of Condensed Matter).

Tong was elected to APS Fellow, 2017.

4.6 Grants

1. K. Yabana, JSPS Grant-in-Aid for Scientific Research (B), 2011-2014, 15,000,000 yen
2. K. Yabana, JSPS Grant-in-Aid for Scientific Research on Innovative Areas, 2013-2014, 3,000,000 yen
3. K. Yabana, JSPS Grant-in-Aid for Scientific Research, 2015-2018, 12,800,000 yen
4. K. Yabana, JST-CREST, 2016-2022, 176,500,000 yen
5. K. Yabana, JSPS Bilateral Joint Research Project, 2013-2015, 4,928,000 yen
6. K. Yabana, Post-K Priority issue 7, Sub-issue B, 2016-2019, 45,900,000 yen
7. K. Yabana, Q-LEAP flagship program, 2018-, 5,000,000 yen
8. K. Yabana, a private company, 2013-2018, 3,150,000 yen
9. K. Yabana, a private company, 2019-, 910,000 yen
10. T. Ono, JST PRESTO, 2013-2016, 30,000,000 yen
11. T. Ono, JSPS Grant-in-Aid for Scientific Research (B), 2016-2019, 11,100,000 yen

12. T. Ono, a private company, 2017, 900,000 yen
13. T. Ono, a private company, 2018, 100,000 yen
14. T. Ono, The University of Tsukuba - DAAD Partnership Program, 2018, 1,497,000 yen
15. X.M. Tong, JSPS Grant-in-Aid for Scientific Research (C),2016-2019, 3,700,000 yen
16. X.M. Tong, JSPS Grant-in-Aid for Scientific Research (C),2012-2015, 4,000,000 yen
17. N. Maeshima, JSPS Grant-in-Aid for Young Scientists (B), 2014-2016, 4,160,000 yen
18. H. Koizumi, ITP/Delta ITP funds, The Netherlands, 2016, 21,175 euro

5 Division of Life Sciences: Biological Function and Information Group

5.1 Overview

All living organisms are composed of simple biological molecules and components such as water, proteins, sugar, RNA, and DNA, which make the highly sophisticated functions, including self-replication, metabolism, homeostasis, and others. In biology, there still remain numerous questions regarding the structures (and/or structural changes) and corresponding functions, and many relevant biological phenomena are not clarified yet. We are interested in elucidating the efficient and complicated biological mechanisms through a time scale longer than a microsecond, and with cooperative motions for large numbers of atoms. Modern experimental methods have remarkably developed biological sciences in the 21st century. We are expecting that theoretical approaches will play an important role in deriving some novel biological findings in the near future because remarkably developments in computer technologies made *in silico* approaches more easily applicable.

For quantitative simulations, huge computational resources are required for most biological systems. Therefore, we have investigated to utilize supercomputers and have been performed realistic computational simulations. Our research areas are focused on the elucidation of reaction mechanisms and physical properties of biomolecules based on molecular mechanics (MM) and quantum mechanics (QM) methodologies and rare event sampling methods based on series of short-time molecular dynamics (MD) simulations. We have mainly elucidated unresolved characters and biophysical mechanisms of biological systems by collaborating with experts in high-performance computer systems, related-fields, and experimental researchers. We are also interested in applying our methods to application fields: photochemistry, drug discovery, and medicines. In particular, we belonged to the photosynergetics project of MEXT, Japan, from 2014 to 2018. We also committed to Post-K computer project of condensed matter physics and astrophysics in collaboration with other researchers in these fields from 2014 to 2019. In this report, we explain the remarkable results in 2014-2019 (fiscal year) in our group.

Member list

The member list of the Division of Life Sciences: Biological Function and Information Group is given below. Since 2014 March, Prof. Shigeta joined and organized the group as the principal investigator (PI). Totally, 1 associate professor, 6 assistant professors, and 8 postdocs joined (currently, 1 associate professor, 3 assistant professors, and 4 postdocs belong to) this group. 2 Ph.D. students, 10 master course students, and 10 undergraduate students graduated from (currently, 1 Ph.D. student, 4 master course students, and 4 undergraduate students belong to) this group. This group accepted one Ph.D. student from Tohoku Univ. (2016-2018) and one master course student from Rikkyo Univ (2019) indicated as (1) in the list.

Name	**2014**	**2015**	**2016**	**2017**	**2018**	**2019**
Y. Shigeta	P	P	P	P	P	P
M. Shoji	A	A	A	A	A	A/JST
M. Kayanuma	A	A	A	A	A	–
R. Harada	PD	PD/JSPS	PD/JSPS	PD/JSPS	A	AP
H. Umeda	PD	PD	–	–	–	–
R. Sato	–	PD	PD	PD	–	–
H. Kitoh-Nishioka	–	–	PD	PD	PD/JST	PD/JST
T.K.M. Bui	–	–	PD	PD	–	–
M. H.N. Al Assadi	–	–	–	A	–	–
H. Nishizawa	–	–	–	–	A	A
Y. Hori	–	–	–	–	–	A
K. Mishima	–	–	–	–	–	PD
Y. Mitsuta						PD/JSPS
K. Hengphasatporn	–	–	–	–	–	PD
Ph.D. Students	0	1	1(1)	2(1)	1(1)	1
Master Course Students	2	1	1	3	4	4(1)
Undergraduate Students	3	1	3	2	2	4

P: Professor; AP: Associate Professor; A: Assistant Professor; PD: Postdoctoral Fellow (PD/JSPS and PD/JST mean the fellowship from JSPS and JST PRESTO, respectively. During this period, PDs were basically independent of PI but belonged and collaborated with the member in this group. Also, A/JST means the assistant professor who is supported by JST PRESTO)

5.2 Research Results

1) QM/MM studies on enzymatic reaction processes

Theoretical elucidations on the reaction mechanisms of enzymes have been performed for many years. In biology, there remain numerous unsolved issues regarding the structural changes, chemical reactions, and signal transduction, which are important not only to construct the fundamental scientific basis but also to develop novel artificial devices. Recently, the rapid progress of X-ray crystallography (XRD), neutron diffraction (ND), electronic microscopy (EM) have taken, and the motions in the catalytic cycles and reliable 3D structures of large protein complexes can be determined. Therefore, elucidations for the structural and energy changes in important and unique biological systems are highly required with tight-collaborations with experimental researchers. On the other hand, for computational progress, both the developments on computational hardware and software-enabled to carry out large-scale molecular simulations. Huge computational resources required for accurate molecular calculations can be directly covered by using supercomputer resources, which are offered by national supercomputer centers such as CCS, Univ. Tsukuba. For the software developments, the validity of the mixed quantum mechanics/molecular mechanics (QM/MM) approach has been confirmed, and rigid maintenances of program packages such as Gaussian, NWChem, Amber, and Gromacs can be utilized. These theoretical approaches and program packages offer sound basics even to construct new methodologies and to develop our original programs and tools.

Enzymatic reactions we have investigated in the past five years from 2014 to 2019 are (1) photosystem II, (2) bilirubin oxidase, (3) heme, (4) threonine synthase, (5), sarcosine oxidase, (6) nitrile hydratase, and (7) nylon-oligomer hydrolase. Here, detailed explanations for the photosystem II, bilirubin oxidase, and nitrile hydrolase are described.

- **Photosystem II: O_2 formation mechanisms in the oxygen evolving complex**

Photosystem II (PSII) catalyzes the water oxidation reaction (WOR: $2H_2O + 4h\nu \rightarrow O_2 + 4H^+ + 4e^-$) using sunlight. This biological catalytic reaction is low-cost and highly efficient as PSII has evolved over 2.7 billion years. Nowadays, the reaction mechanisms of the natural WOR attract significant attention not only for biological importance but also for developing advanced artificial photosynthesis. Therefore, WOR has been intensively investigated internationally and in many different research fields such as inorganic chemistry, nanoscience, and quantum physics. The catalytic reactions of the oxygen-evolving complex in photosystem II (PSII-OEC) are known as the Kok-Joliot cycle, and their five states are named as S_i (i=0-4) for the accumulated oxidation states. It has been expected that the important chemical reactions are carried out in $S_2 \rightarrow S_3$ and

$S_3 \rightarrow S_0$ transitions, in which the largest structural change is performed for the Mn cluster, and the molecular dioxygen (O_2) is formed. However, a variety of chemical reactions have been proposed in the past decades, and it is not easy to compare the stabilities among different mechanisms without using a large theoretical model. We have found that the stabilities of intermediate states (S_0, S_1, S_2, and S_3 states) can be precisely evaluated by using large scale QM/MM models (Figure 1), and experimental results can be reproduced well. We have also elucidated the early stage reaction mechanism in the $S_2 \rightarrow S_3$ transition. Theoretical elucidations for the $S_3 \rightarrow S_4 \rightarrow S_0$ transition at highly accurate theoretical levels are also performed. We proposed new mechanisms for the O-O bond formation mechanisms. One is a Non-Adiabatic One-electron Transfer mechanism (NA-OET), and another is a Concerted Bond Switching (CBS) mechanism, which is carried out via non-radical electronic structures. We also clarified that O_2 release and water insertion in the $S_3 \rightarrow S_0$ transition must occur concertedly. After our theoretical reports, XFEL structures by Barkley and Okayama groups independently were reported for the S_2 and S_3 states. Reaction rate experiment using a Val185Thr mutation by Sugiura *et al.* reported that the $S_3 \rightarrow S_0$ transition is drastically decreased. These experimental results are consistent with our fist theoretical proposals for the $S_2 \rightarrow S_3$ and $S_3 \rightarrow S_0$ transitions. By utilizing supercomputer facilities such as K computer, COMA, and OFP, the most important chemical reactions in PSII-OEC have been reported. Our research results will be valuable not only for the biological

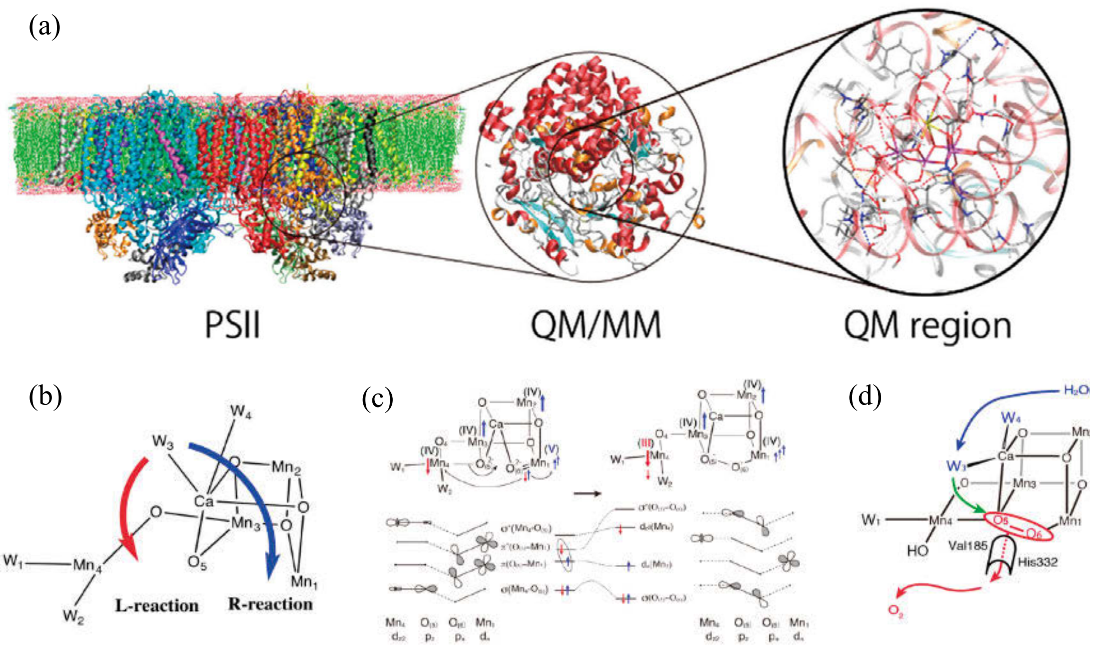

Figure 1. (a) Structure of PSII, large scale QM/MM model for the PSII-EC and the QM atoms, (b) first water insertion pathways in the S_2 -> S_3 transition, (c) concerted bond switching mechanism proposed as a new non-radical O-O bond formation mechanism in PSII-OEC, and (d) concerted process for the O_2 ejection and the second water insertion in the S_4 -> S_0 transition.

importance but also to realize clean and highly efficient artificial photosynthesis as the same chemical reactions should be carried out efficiently.

- **Bilirubin oxidase**

Bilirubin oxidase (BOD) catalyzes the bilirubin oxidation using the reduction of dioxygen into the water: 2 bilirubin + O_2 + 4 H^+ → 2 biliverdin + 2 H_2O. BOD belongs to the family of multicopper oxidases (MCOs), which contain unique Cu atoms, i.e., type 1 copper (T1Cu), type 2 copper (T2Cu), and type 3 copper (T3Cu). The O_2 reduction is carried out at the trinuclear Cu center (TNC), which is composed of one T2Cu and a pair of T3Cu atoms, T3aCu and T3bCu. T1Cu plays an essential role in electron transfer from the substrate to TNC. The BODs have been widely utilized for the diagnostic analysis of bilirubin in serum. Recently, BODs have attracted attention for use as an enzymatic catalyst for the cathode of biofuel cells because of the high activity at neutral pH. Geometric and electronic structure changes in the copper (Cu) centers in bilirubin oxidase (BOD) upon a four-electron reduction were investigated by QM/MM calculations (Figure 2). We found new candidates of the native intermediate and the resting oxidized states. Elongations of the Cu-Cu atomic distances for the trinuclear Cu center (TNC) and very small structural changes around the type I Cu (T1Cu) were calculated as the results of a four-electron reduction. The QM/MM optimized structures are in good agreement with recent high-resolution X-ray structures. As the structural change in the TNC upon reduction was revealed to be the change in the size of the triangle spanned by the three Cu atoms of TNC, we introduced a new index (*l*) to characterize the specific structural change. Not only the wild-type, but also the M467Q, which mutates the amino acid residue coordinating T1Cu, were precisely analyzed in terms of their molecular orbital levels, and the optimized redox potential of T1Cu was theoretically reconfirmed.

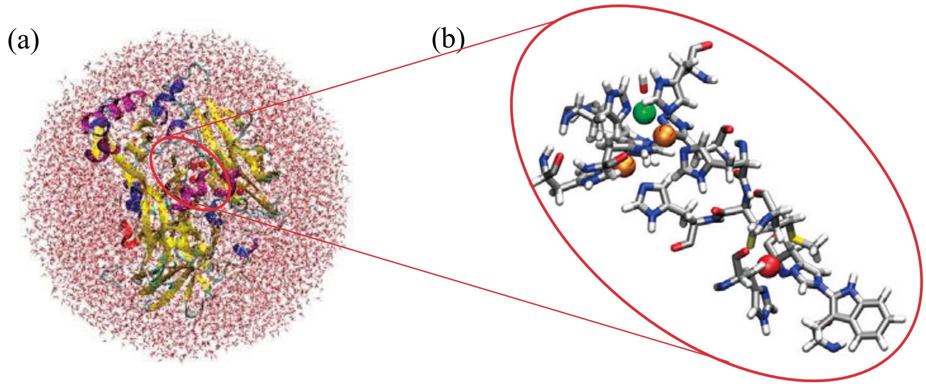

Figure 2. (a) Overall view of the bilirubin oxidase. (b) QM region used for the QM/MM calculations. MM region is not shown for clarity.

- **Nitrile hydratase**

Nitrile hydratase (NHase, Figure 3) catalyzes the hydration of nitriles to the corresponding amides (R-CN + H_2O → R-$CONH_2$) and is widely used in the chemical industry for the production of acrylamide. We investigated the reaction mechanism of NHase containing an Fe(III) ion at the active site using the QM/MM method. First, we analyzed the initial steps of the catalytic mechanism. We examined four possible reaction paths and showed that the formation of a cyclic intermediate is the most probable one. The result is consistent with previous experimental and theoretical (cluster model) studies. Then, we analyzed the reaction mechanisms subsequent to the cyclic intermediate and revealed the details of the catalytic reactions of NHase, which proceeds via disulfide and imidic acid intermediates. We also shed light on the role of an amino acid residue (βArg56) by analyzing the reaction of a mutant. In addition, it was shown that the explicit treatment of the protein environment, which had been considered using PCM in previous theoretical studies using cluster models, is important to analyze the reactions of NHase.

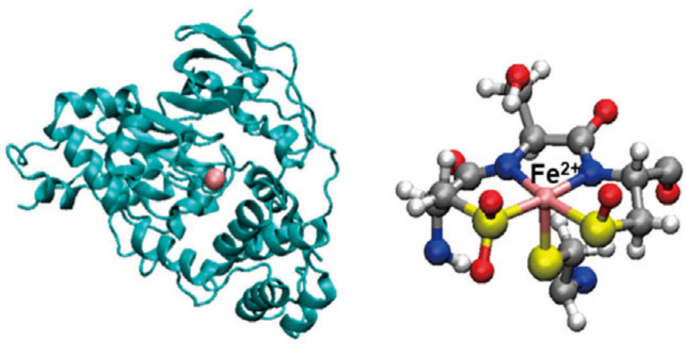

Figure 3. Whole (left) and active site (right) structures of the Fe-containing NHase.

2) Molecular dynamics studies on structural transition of proteins

- **Developments of Rare Event Sampling Methods for Understanding the Biological Functions**

The biological functions of proteins are strongly related to their conformational transitions. To elucidate the essential dynamics, molecular dynamics (MD) simulation has become a powerful tool. However, it might still be difficult to address the relevant conformational transitions of proteins with the conventional MD (CMD) simulations because the accessible time scales of CMD simulations are far from those of the biological functions. Furthermore, the essential transitions are induced as stochastic processes in the long-time scales, i.e., the conformational transitions of proteins are regarded as *biologically relevant rare events*. To reproduce/predict the rare events, we have proposed a variety of rare event sampling methods. Our strategy to detect the rare events is based on cycles of the following conformational resampling consisting of two steps. (1) Selections of essential initial structures. (2) Restarting of short-time MD simulations from the initial structures. The cycles of simple conformational resampling increase the transition probabilities, promoting the rare events. Our conformational sampling methods are rather simple. Basically, all the methods adopt a common strategy for the conformational sampling. The flowchart of the common conformational sampling is shown in Figure 4. In our methods, cycles of the following conformational resampling are repeated to promote the conformational transition of a given protein. Herein, the procedure of the conformational resampling is briefly described below.

1. Performing short-time (typically ps−order) MD simulations from the initial structures (n_{initial} = 10−100) under a canonical ensemble (*NVT* or *NPT*), where n_{initial} is the total number of initial structures.
2. Ranking the structures of short-time MD trajectories based on a predetermined rule (selection rule).
3. Selecting the initial structures at the next cycle so that snapshots of a higher rank are preferentially selected.
4. Regenerating initial velocities of a given target temperature based on the Maxwell − Boltzmann distribution in restarting the short-time MD simulations from the initial structures.
5. Repeating the cycles of (1)−(4) until the obtained distribution along initially specified RCs does not change anymore. Otherwise, the cycle ends when the desired distribution is obtained. A criteria to terminate the cycle of the conformational resampling depends on each method.
6. Evaluating the obtained transition paths on a free energy landscape (FEL). Applying the umbrella sampling method followed by the weighted histogram analysis method to estimate the FEL projected on reaction coordinates (RCs) in terms of the transition path obtained above. The Markov state model (MSM) is also

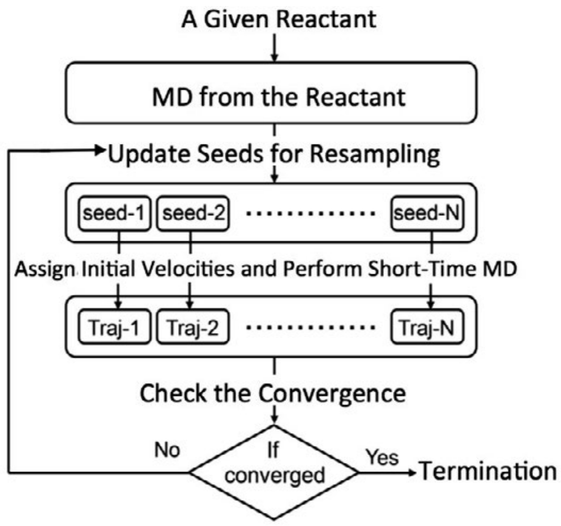

Figure 4. Common design concept of our rare event sampling methods. Initial structures (seeds) for the first cycle (seed-1, seed-2, ..., seed-*N*) are generated with short-time MD simulations from a given reactant. Then multiple trajectories generated by conformational resampling (Traj-1, Traj-2, ..., Traj-*N*) are gathered and utilized to update (*N*) seeds at the next cycle. To promote the structural transitions for a given protein, cycles of the conformational resampling are repeated. The initial velocities are regenerated based on the Maxwell-Boltzmann distribution when restarting the short-time MD simulations.

utilized to estimate the FEL with a transition matrix by counting the transitions among defined microstates.

In our methods, the selection of reasonable initial structures might be essential to make transitions. Among all the methods, only the selection rule of initial structures in (2) is different. Except for the free energy calculation in (6), the conformational resampling from (1) to (5) can be easily performed without modifying MD programs. In actual applications, cycles of the conformational resampling can be controlled with simple scripts. Therefore, our methods are simple, yet efficient/powerful for reproducing/predicting the conformational transitions relevant to the biological functions. Herein, we review the enhanced conformational sampling methods developed by us, i.e. (A) parallel cascade selection MD (PaCS-MD), (B) fluctuation flooding method (FFM), (C) taboo search algorithm (TBSA), (D) outlier flooding method (OFLOOD), (E) structural dissimilarity sampling (SDS), and (F) self-avoiding conformational sampling (SACS).

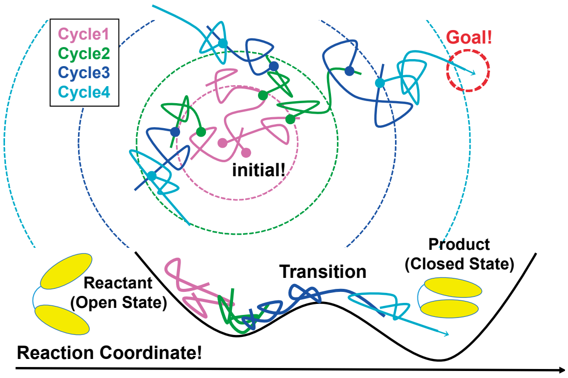

Figure 5. The concept of parallel cascade selection molecular dynamics (PaCS-MD). To promote conformational transitions from a given reactant to a product, cycles of conformational resampling consisting of (1) selections of initial structures and (2) restarting of short-time MD simulations are repeated. In PaCS-MD, structures close to the product are always selected and resampled by restarting of short-time MD simulations, making a transition to the product efficiently.

As a representative conformational sampling method, we would like to introduce PaCS-MD. PaCS-MD is a conformational sampling method for generating a set of transition paths from a given reactant to a product under the condition that the end-point structures are known *a priori*. Figure 5 shows a flowchart of PaCS-MD. By repeating a cycle of the conformational resampling, PaCS-MD generates possible conformational transition paths from the reactant to the product. As an RC to measure the structural similarity to the product, a root-mean-square deviation from the product ($RMSD_{product}$) is the most general choice. At the end of each cycle, all the structures of trajectories are ranked by $RMSD_{product}$. In the process of ranking, structures with small $RMSD_{product}$ values are selected among all the trajectories and are adopted as the reasonable initial structures to be resampled at the next cycle. The cycles of conformational resampling are repeated until highly ranked structures reach the product, i.e., $RMSD_{product}$ < cutoff, where the cutoff is a threshold for terminating the PaCS-MD cycle. Finally, a sufficient PaCS-MD cycle provides a set of conformational paths between the end-point structures.

3) Astrobiology

Astrobiology is a new scientific field that closely relates to astrophysics, biology, chemistry, and space science. Recently, as the progress on the detection technologies and methods have been developed significantly and observations of extrasolar planets have been reported one after another. For example, many candidates within the habitable region and close ones (Proxima Centauri b, 4 light-years away from Earth) have been found out. Therefore, the ultimate mystery for the origin of life such as "how life on Earth was created?" and "is life universal outside on Earth?" will be solved. Before trying these issues, we have first tried to elucidate how glycine, the simplest amino acid, can be formed in the interstellar medium (ISM). Glycine has been one of the major targets in the search for prebiotic molecules in the ISM, although glycine has not been detected. It is noted that glycine was certainly detected in meteorites. Therefore, we wanted to clarify which formation pathways can be expected for the glycine formation.

- **Glycine formation in extraterrestrial environments: reactions from stable molecules**

First, possible reaction paths for the formation of glycine in extraterrestrial environments called Strecker-type and Bucher-Bergs reactions were investigated by means of the DFT method. We examined the formation of hydantoin from aminoacetonitrile and the hydrolysis of hydantoin to generate glycine. Aminoacetonitrile and hydantoin are detected in an interstellar cloud and meteorites, respectively. However, reaction barriers for the proton transfers and bond formation reactions over 210 kcal/mol. This activation barrier is too high for reactions in IMS of about T = 10K-100K, even considering the catalytic effects of water molecules on interstellar ices (Figure 6). This means that these reactions do not occur even at the time scale of about 10^6 years. Thus, some energy sources are required for proceeding the reactions, such as the heating of the meteorite parent body.

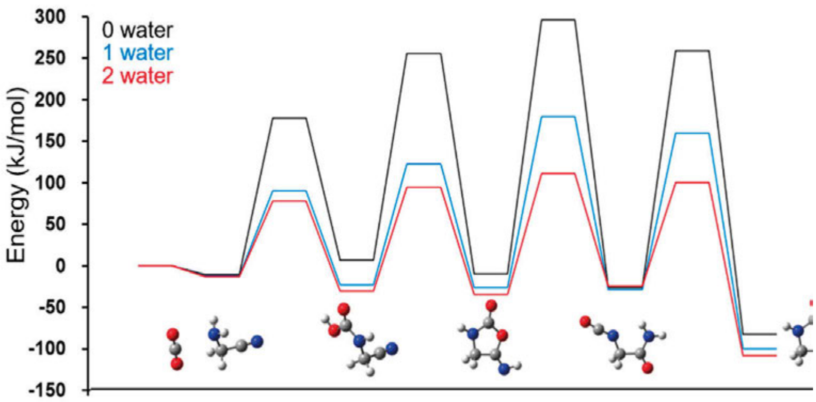

Figure 6. Energy profile of the formation of hydantoin from aminoacetonitrile with 0, 1, or 2 catalytic water molecule(s).

- **Glycine formation in extraterrestrial environments: radical coupling reactions**

Next, we investigated the radical coupling processes proposed by Garrod in 2013. Based on his results by the chemical network model, three routs dominant in 40 K < T < 55 K, 55 K < T < 75 K, and $T\rightarrow$ 75 K temperature ranges are investigated. These routes contain NH_2CH_2CO and OH radicals, NH_2 and CH_2COOH radicals and NH_2CH_2 and HOCO radicals to form glycine, respectively. Among these routes, first and third routs are clarified to be almost barrierless, on the other hand, the second route requires 33.41 kJ/mol in the hydrogen subtraction process from CH_3COOH to ・CH_2COOH radical. Therefore, we concluded that the radical process is a most candidate for the glycine formation, though the second rout is unlikely compared to the first and the third reaction pathway. As the glycine formation process proceeds thorough reaction between precursors, reactions over adsorption and condensation process are important. We also discussed about the origin of heavy atoms in glycine.

4) Computational Biomolecular Medicine

- **Developments for Predicting Membrane Permeation Processes of Cyclic Peptides**

To design rational drugs, it is important to evaluate membrane permeations because they penetrate cells from the outer to inner membranes as their functions. However, the membrane permeation is difficult to measure experimentally with the high resolution because of the structure of lipid bilayers are complicated. In contrast, computational approaches, as represented by molecular dynamics (MD) simulations, might provide atomistic-level insights of membrane permeation. Also, MD simulations can address the essential interactions of drugs with membranes. Therefore, it might be the first step to generate the membrane permeation processes of small (cyclic) peptides. As a final step, free energy profiles upon the membrane permeations will be a goal for understanding their mechanisms in rational drug design. However, conventional MD (CMD) is inappropriate for catching the membrane permeations that involve high energy barriers, i.e., the membrane permeation processes are induced in an extremely long-timescale as rare events. Therefore, it is quite difficult to catch the rare events with CMD simulations. To catch the membrane permeation processes, one must perform extremely long-time MD simulations. To solve the sampling problem, several accelerated sampling methods that bias the system to sample inaccessible conformational subspaces have been proposed. In contrast to the so-called biased sampling methods, we have proposed non-biased sampling ones. Parallel cascade selection MD (PaCS-MD) is a representative example of the non-biased methods developed by us (see Sec. 5.2 2) for the detail of PaCS-MD).

Herein, we have utilized PaCS-MD to catch the membrane permeation processes of cyclic peptides using a simple (POPC) lipid bilayer system. The concept for catching the rare membrane permeation processes based on PaCS-MD is shown in Figure 7. PaCS-MD repeats conformational resampling from important initial configurations of cyclic peptides, i.e., PaCS-MD always selects relevant configurations of cyclic peptides with high potentials to penetrate cells by referring to the permeation direction, and restart shot-time MD simulations from the selected configurations. By repeating cycles of conformational resampling, PaCS-MD gradually catches the membrane permeation without any external (biased) forces as shown in Figure 7. In the current status, we have successfully generated a set of membrane permeation processes of a simple cyclic peptide for the POPC lipid bilayer. As a next step, we would like to evaluate free energy profiles upon the permeation processes of these peptides by constructing reliable Markov state models in terms of the PaCS-MD trajectories.

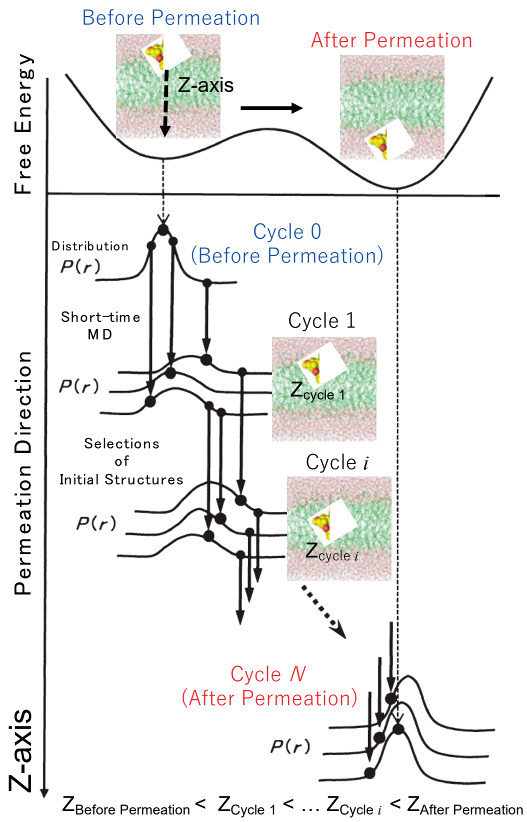

Figure 7. Concept of PaCS-MD for predicting membrane permeation processes on a lipid bilayer.

5) Photosynergetics Project of MEXT.

- **Triplet-triplet Annihilation Up-conversion (TTA-UC) in liquid and solid phase**

Recently, the triplet-triplet annihilation (TTA) based photon up-conversion (UC) process has been extensively studied as a possible device that utilizes solar power because TTA-UC generates high-energy photon emission from absorptions of lower energy photons. One of the most remarkable advantages of TTA-UC over the other UC processes using multiphoton absorptions, f-f transitions of rare-earth elements, and so on, is that TTA-UC occurs even with the solar light intensity (~100 mW/cm^2). Thus, the investigation into design principles for developing robust TTA materials is of great importance. However, TTA-UC process is quite complicated. Thus, one should analyze a series of these processes in parallel to deeply understand the mechanism of TTA-UC. In many experiments, platinum or palladium octaethyl porphyrin (PtOEP or PdOEP) and

9,10-diphenylanthrance (DPA) have been selected as the sensitizer and emitter, respectively and achieved the high TTA-UC quantum yield (QY) (26%) in solution. However, in theoretical analysis, there are many studies for the TTET processes, but not for the TTA processes. Thus, the present study focuses on the clarification of TTA processes using the theoretical methods.

TTA is driven by an electron exchange mechanism generated charge separation between two triplet emitters as shown in Figure 8. For each step in Figure 8, the electron transfer (ET) rate can be estimated by the Marcus formula. To evaluate electron coupling matrix elements, T_{DA}, for the TTA, we have adopted the fragment molecular orbital (FMO) method and FMO-liner combination molecular orbital (FMO-LCAO) methods. We have developed the calculation methods for TTA processes in solution based on Marcus theory and analyzed TTA rate constants. We also used the same methodologies for TTA processes in solid phase. For the solution phase, the TTA reaction time τ (the inverse of the TTA rate) of the dimer models of 9,10-diphenylanthracene (DPA) and the alkyl-strapped derivatives (C*n*-sDPAs) was evaluated. The τ for the C*n*-sDPAs was much shorter compared to that of DPA even at long distances and at various mutual orientations of the dimers. This shortened τ was due to the large electron coupling matrix elements through the pseudo-π-orbital that was extended to the alkyl chains in the singly occupied orbitals. This finding supports the observed superior performance of TTA upconversion obtained with C*n*-sDPAs. For the solid phase, the TTA reaction time τ_{TTA} and triplet-triplet energy transfer (TTET) time τ_{TTET} of all neighboring pairs of DPA and C7-sDPA were compared. It was found that the dimensionality of them is of great importance in the efficiency of the TTA up-conversion process in the solid phase compared to those in the solution phase since the molecular packing in crystalline is almost unchanged and the orientation of molecules is fixed in the solid phase. Thus, the synergetic effect of TTA and TTET processes is one of the key factors for highly efficient TTA-UC materials.

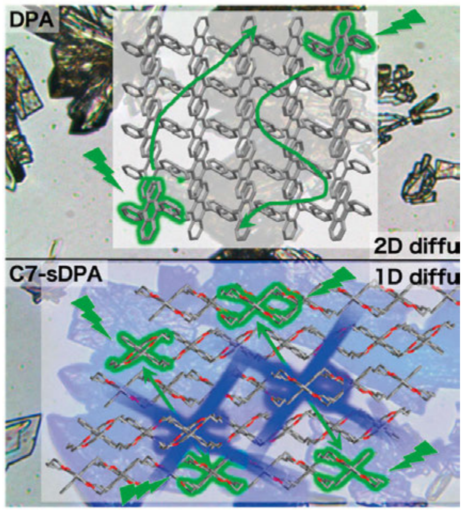

Figure 8. Schematic view for diffusion of triplet exciton in DPA and C7-sDPA crystals.

- **Excited-state Aromaticity**

The aromaticity of photoexcited molecules is an important concept in organic chemistry. Its theory, Baird's rule for triplet aromaticity gives the rationale of photoinduced conformational changes and photochemical reactivities of cyclic π-conjugated systems. However, it is still challenging to monitor the dynamic structural change induced by the excited-state aromaticity, particularly in condensed materials. Here we report the direct structural observation of molecular motion and a subsequent packing deformation accompanied by the excited-state aromaticity. Photoactive liquid crystal (LC) molecules featuring a π-expanded cyclo-octatetraene core unit are orientationally ordered but loosely packed in a columnar LC phase, and therefore a photoinduced conformational planarization by the excited-state aromaticity has been successfully observed by time-resolved electron diffractometry and vibrational spectroscopy. The structural change took place in the vicinity of excited molecules, producing a twisted stacking structure. We have analyzed structures and their changes using theoretical methods, and compared with the experimental results to confirm the excited-state aromaticity. A nanoscale torque driven by the excited-state aromaticity can be used as the working mechanism of new photo-responsive materials.

6) Post K-computer Project of MEXT

- **First principle analysis of ammonia adsorption and desorption on GaN surface**

Gallium nitride (GaN), which belongs to the III-V family, is attracting tremendous attention recently since GaN is used in optoelectronics, photonics, high power and high-temperature operation devices owing to having wide-bandgap. Metal Organic Vapor Phase Epitaxy (MOVPE) with trimethylgallium (TMG) and ammonia (NH_3) as gas sources is regarded as the most suitable technique of growing GaN films. Many experimental and theoretical efforts have revealed that TMG is decomposed in the gas phase, and the growing surface is generally Ga rich. Knowledge of the decomposition and incorporation of NH_3 is, however, extremely poor. Using the density functional theory (DFT) method, as implemented in real-space density functional theory (RSDFT), we aim to theoretically investigate reaction mechanisms of ammonia on (0001) GaN surface for understanding the elementary process in the crystal growth. The

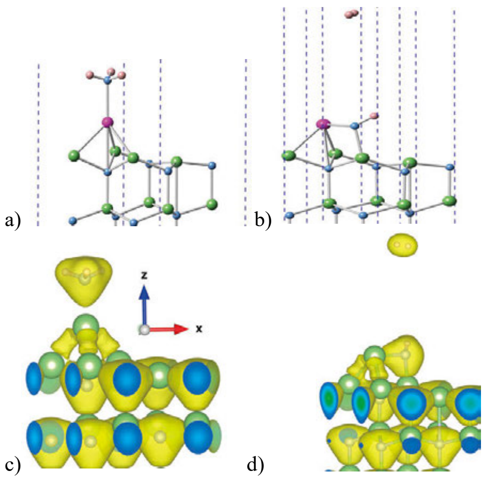

Figure 9-1. The initial (a) and the final (b) atomic structures of the decomposition reaction of NH_3 and the corresponding charge density (c), (d). Large and small balls depict Ga and N atoms, respectively.

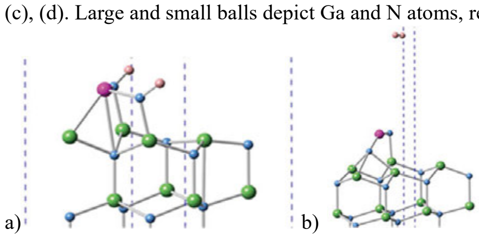

Figure 9-2. The initial (a) and the final (b) atomic structures of the decomposition reaction of NH.

calculated lattice parameters for bulk (a = 3.2 Å, c = 5.2 Å) are in accordance with experiments. After identifying the growing surface, which is Ga rich in general, we have determined the adsorbed structure of NH_3 on the Ga rich surface. On the Ga-rich surface, relatively weak Ga-Ga bonds exist as shown in Figure 9. We have indeed found that the reaction, [NH_3 on GaN] → [NH in GaN] + [H_2 in gas phase], takes place with the energy barrier of 0.48 eV. After this reaction, N in NH_3 intervenes in the weak Ga-Ga back bond, forming the network of –Ga adatom – N(H) – Ga –. Then we have explored the possible reaction when this configuration is formed at the same Ga-adatom site. We have found a reaction pathway in which two H atoms in the two NH units get together and desorbed in the gas phase, and the remaining N atoms form Ga-N bonds. One of the two N atoms even becomes 4-fold coordinated with neighboring Ga atoms as shown in Figure 9, thus forming a new basic unit constituting the GaN film. The energy barrier for the reaction is found to be lower than 1.5 eV at zero temperature.

- **First-principles calculations of Na ion containing transition metal oxides**

Establishing technologies such as long-distance travel by electric vehicles and megawatt storage of renewable energy sources requires high-performance batteries. Conventional Li-ion charge carriers are likely to be severely restricted in the future because lithium resources are scarce and unevenly distributed throughout the earth. On the other hand, the use of Na ions as a substitute for Li is also promising, but there are many challenges. For example, since Na has a larger ionic radius and a smaller ionization potential than Li, the energy density of a Na-based cathode decreases. Therefore, bringing the Na ion-based cathode to the Li level requires careful adjustment of all performance enhancement mechanisms.

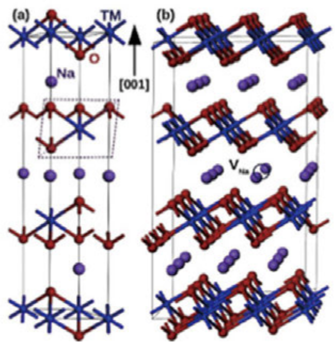

Figure 10. Structure of Na ion-containing transition metal oxides (a) and its vacancy model (b).

In this study, the density-functional band calculation of the sodium-containing transition metal oxide ($NaTMO_3$) containing the transition metal (TM) in the 4th to 5th period with the structure shown in Figure 10. The electrode potential was evaluated from the energy difference between the state and the reduced state. From the calculation results, it was shown that the measured value was well reproduced for the solution with the measurement result. It was also revealed that rather than the ionicity of the TM-O bond, the cathodic potential is governed by the distortion of oxygen coordination around the TM due to oxidation and the accompanying magnetic exchange interaction. Through this research, we proposed a design guideline based on the electron configuration of transition metal and its change instead of the conventional material design guideline based on ion or potential.

7) Development of Software

- **GPU acceleration of Fragment Molecular Orbital (FMO) method**

Fragment molecular orbital (FMO) method is a representative method of large-scale electronic structure calculations for biomolecules, such as a protein. OpenFMO is an open-architecture program for the large FMO calculations on the petascale massive-parallel computing systems through the MPI+OpenMP hybrid parallelization scheme. Toward the FMO calculations on the exascale computing systems with modern NVIDIA graphics processing units (GPUs), we have developed a GPU-accelerated OpenFMO program, done some benchmark calculations, and made its source code publicly available on GitHub at https://github.com/OpenFMO/OpenFMO.

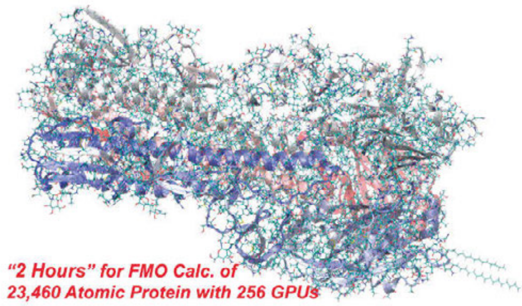

Figure 11. Influenza HA3 protein (721 fragments, 2 residues/ fragment).

We implemented the GPU-enabled kernel codes in the bottle-neck parts of the OpenFMO program: the 4C-IFC (four-center two-electron integrals involved in inter-fragment Coulomb interactions) and Fock-matrix construction. Both the parts include the time-consuming two-electron (2e) integral calculations and involve accumulating them to the shared matrices. Because the accumulation usually needs massive slow "atomic" (exclusive addition) operations, we have developed a novel parallelization algorithm to avoid the operations.

For one of the benchmark calculations, we did the FMO2-RHF/6-31(d) calculations of the influenza HA3 protein (Figure 11) on the HA-PACS GPU Base Cluster system. In the calculations, we used 64 nodes with 256 GPUs (NVIDIA Tesla M2090). As a result, our GPU-accelerated OpenFMO completed the FMO calculation of HA3 within only 2 hours.

We made the GPU-accelerated OpenFMO program publicly available through an open-source MIT license. We have re-designed and re-created the OpenFMO official web site, https://openfmo.org, which provides further detail information, including how to download, compile, and execute it with command-line options, and several examples used as a tutorial and template for the users. We are now continuing to extend the range of its application. We have newly implemented DFT (density functional theory) code in OpenFMO program. We also succeeded in the FMO-B3LYP/6-31G(d) calculations of HA3 (Figure 11). However, it took ca. 12 hours because we didn't complete the GPU-enabled kernel code for evaluating the exchange-correlation term in DFT calculations. The RI-MP2 (resolution-of-identity MP2) extension of the GPU-accelerated OpenFMO is another crucial task toward advanced in-silico drug design. We will distribute the extended OpenFMO programs through the official web site.

- **Density Functional Tight-Binding Molecular Dynamics (DFTB-MD) Simulation**

The molecular dynamics (MD) simulation based on the density-functional tight-binding (DFTB) method, which is one of the semi-empirical quantum mechanics (QM) techniques, becomes applying to the biomolecular systems. In the MD simulation, the amount of simulation sampling and the energy conservation affect the accuracy of properties. Although the time series of the total energy is known to good conserve in the classical MD simulations, there were few assessments of the energy conservation for the DFTB-MD simulations. Thus, we verify the energy conservation of the DFTB-MD simulations. Furthermore, to accelerate DFTB-MD simulations, we applied to the constraint technique, namely RATTLE, to the DFTB-MD technique. Since the conventional RATTLE technique needs many times of iterative procedures, we reduce the iterative procedures by newly deriving the matrix form of RATTLE technique.

First, the matrix form RATTLE technique was applied to the water molecule. The conventional RATTLE technique needed 27 cycles to constrain all distances of the water molecule, i.e., the distances of O-O and two O-H, from a random structure. On the other hand, our matrix form RATTLE needed only 3 cycles. Therefore, newly developed RATTLE method is about 9 times faster than the conventional RATTLE. Next, the DFTB-MD simulations with RATTLE technique were carried out for 64 methanol molecules. When the time step was set to 0.5 fs, the total energies of DFTB-MD simulations conserved whether RATTLE was applied or not. However, when the time step was set to 1.0 fs, the total energy did not conserve in the DFTB-MD w/o RATTLE. On the other hand, in the DFTB-MD w/ RATTLE, the time step was able to increase 2.0 fs to conserve the total energy. Therefore, we confirmed that the time step must be set to 0.5 fs in the normal DFTB-MD simulations, and the DFTB-MD simulation can be accelerated 4 times using the constraint technique.

- **GPU acceleration of Car-Parrinello Molecular Dynamics (CPMD) method using real-space density functional theory (RSDFT).**

The real-space density functional theory (RSDFT) developed by one of us has enabled static calculations of several tens of thousands of silicon atoms on K computer [See Y. Hasegawa *et al.*, *J. High Perform. Comp. Appl.* **28**, 335 (2014). and https://github.com/j-iwata/RSDFT.]. However, in order to describe the physical properties of a given system, entropic contribution becomes important as the number of particles increases. Molecular dynamics (MD) simulations are usually used to take it into account. However, it is difficult to handle chemical reactions with classical

MD. Nevertheless, the first-principles MD (FPMD) also has a drawback in required computational costs. In order to avoid them, Car and Parrinello have proposed an efficient method to avoid solving the self-consistent field calculations in FPMD [R. Car, M. Parrinello, *Phys. Rev. Lett.* **55**, 2471 (1985)].

We have implemented CPMD modules in RSDFT (RS-CPMD), which enables us to simulate a thousand atoms FPMD on K computer. Here, the performances of a GPU version of RSCPMD under the support of ISSP (SGI Japan and Ark Information Systems) are presented. The most severe bottleneck in RS-CPMD is the evaluation of inner products between wave functions and its velocities ($O(N_{grid}^3)$). Therefore, in the implementation of the last year, we made GPU modules for this inner product calculation. Since BLAS3 routines can be used for this operation, three or four-fold speed-up can be achieved by adopting GPU. In this year, GPU versions of several routines in a force evaluation were implemented. By changing the numbers of MPIs and threads, we have tested our programs on ISSP system B 64 nodes (512 cores and 128 GPUs) for an organic solvent (1664 atoms) as a target system. For the fastest case, it took 6.28 sec for one CPMD step, which is comparable with 5.54 sec with 4096 cores in K computer. For Ewald and local force calculations, drastic speed-up was achieved, while the performance of the GPU version for non-local forces is not high due to a difficulty in load balance and multiple internode communications.

5.3 Collaboration

1) Collaboration within Division of Life Sciences

We are collaborating with Profs. Y. Inagaki and T. Hashimoto in the Molecular Evolution Group to investigate protein-protein interactions of translation elongation factors in eukaryotes and published one paper about it in 2019.

2) Collaboration with Division of High Performance Computing System

In order to develop the hybrid MPI/OpenMP and mixed GPU parallelization of a fragment molecular orbital method, we are in close collaboration with members of the Division of High-Performance Computing System (HPCS). Drs. H. Umeda and H. Kito-Nishioka, post-doctoral fellows under the support of a CREST project (Research director, Prof. T. Boku), developed the GPU-accelerated FMO with the help of HPCS groups. We have published two papers and one book chapter concerning about GPU-accelerated FMO programs. Currently, we have started the GPU-FPGA implementation of CPMD with RSDFT for further acceleration in the force calculation.

3) Collaboration with Division of Astrophysics

Astrobiology studies have been performed with collaborations with Prof. M. Umemura, Prof. K. Ohsuga, Assoc. Prof. H. Yajima, Assis. Prof. K. Furuya (the Division of Astrophysics), Prof. K. Shiraishi (now in Nagoya University), Prof. K. Yabana (the Division of Quantum Condensed Matters Physics), and Prof. Y Aikawa (now in University of Tokyo). We performed the first-principles calculations for synthetic pathways of biomolecules in space astronomical environment. Currently, we have published five papers about astrobiology and still collaborated with several groups in CCS.

4) Collaboration within Computational Medical Sciences

Since 2018, we have started collaboration in the computational medical sciences with Profs. M. Umemura, H. Kitagawa, and I. Kitahara. We have held the symposiums of the computational medical sciences twice in 2018 and 2019 together with them.

5) Collaboration with other institutes

Since 2017, Prof. Shigeta became a visiting professor of the Institute for Space and Astronautical Sciences (ISAS), Japan Aerospace Exploration Agency (JAXA). He and his partners have held several joint lectures and discussions about "astrobiology" once a month until the 2020 fiscal year. He also became a visiting researcher of the National Institute for Quantum and Radiological Science and Technology (QST) since 2018. He collaborated with the biophysicists working in the neutron crystallography at Japan Proton Accelerator Research Complex (J-Parc) and had discussions about "quantum biology" twice a year.

5.4 Future Plan

The division of life sciences: biological function and information group continue the fundamental researches on investigating the relationship between structures and function at the atomic level by using QM, QM/MM, and MD simulations. The detailed plans for each topic are listed below. On the other hand, the MEXT projects for the photosynergetics and for the Post K computer have been finished. Instead, we will propose alternative projects concerning the biophysics and biochemistry.

1) QM/MM and QM analyses on Metalloproteins

Living organs constantly maintain their system by taking in substances from the outside, extracting energy from them, and converting them into various forms of energy. In particular, various metalloproteins are involved in energy conversion, and thus understanding enzymatic reactions is the key to answer the question "What is life?". For this purpose, we have developed theoretical methodologies for investigating bioenergetics based on (chemical) thermodynamics and electrochemistry, and the energetics of biological systems can be quantitatively determined through physical quantities obtained by first-principles (quantum chemical) calculations such as free energy changes during enzymatic reactions, pK_a and redox potential, and so on. During the next 6 years, we also continue the first-principles calculations of biologically relevant metalloproteins such as, PS-I and PS-II (supported by PREST, JST), Hydrogenase (by "Hydrogenomics", a project of Innovative area JSPS, Japan), and DNA photolyase and phycocyanin (by "Molecular Movie", a project of Innovative area JSPS, Japan).

2) Molecular Dynamics simulations for biological systems

Nowadays, simulation techniques such as MD, Monte Carlo (MC), and others are widely applied to predict the three-dimensional structure of proteins in principle, elucidating the mechanism of enzyme reactions, and theoretically designing drugs. However, the biological processes occur in a timescale extremely longer than that can be reached by CMD simulations. To overcome the drawback, we have established a series of enhanced sampling techniques named PaCS-MD and applied it to several problems such as protein-folding, large-amplitude domain motions, and so on.

Using the PaCS-MD simulations, we will perform several applications to understand the structure (change)-function relationships of biological molecules. Especially, we are currently interested in the liquid-liquid phase separation of Fused in Sarcoma (FUS) proteins, off-target effects of CRISPR-Cas9, and an activation process of C-terminal binding proteins. Also, we collaborate with members of several projects upon request. We also extend the free energy estimation method using the Markov state model with PaCS-MD to reduce further the computational costs in searching the structural transition and calculating the free energy barrier.

3) Integrated MD and QM methods for the rational design of middle-sized molecular drugs

In recent years, attention has again been paid to middle(medium)-sized molecules (molecular weight is in a range of 500-1000) such as natural products and non-natural and/or unconventional peptides such as cyclic peptides including D-type amino acids since they can be precisely synthesized by chemical synthesis (partially biosynthesis) like as conventional small-sized drugs. Drug discovery targeted on the peptide and nucleic acid has been studied for a long time. However, they suffer from degradation by resident enzymes such as peptidase and nuclease in the human body. On the other hand, cyclic peptides and D-amino acids are resistant to peptidase degradation. Moreover, the former overcomes some of the problems of conventional antibody such as superior membrane permeability by chemically introducing substituents. However, the optimal reaction routes, cell permeation, and how such medium-sized molecules have pharmacological activity have not been clarified yet.

In the next 6 years, we go on researches on reaction path analysis using first-principles calculations and analyses of membrane permeation processes, $LogP_{o/w}$, and substrate-protein binding processes using molecular dynamics calculations for drug discovery targeting on medium-scale molecules. In addition, we will develop theoretical methodologies and programs for them by using the supercomputers in CCS and apply them to natural and non-natural lead compounds (under the support by the Middle-sized molecular drug project, Agency for Medical Development (AMED) until the 2020 fiscal year).

4) Astrobiology

One of the main issues in astrobiology is the origin of matter and life in the universe. However, it is impossible to reproduce the formation of the universe and stars by experiments, and it is necessary to make *a priori* judgment based on experimental facts, theories, and calculations currently available. Therefore, theoretical calculations are becoming increasingly important. In particular, in the chemical evolution process of matter in the interstellar molecular cloud, which is the stage of star and planet formation, the multiscale problem of matter formation and dissociation in molecular clouds, ice surfaces, and cosmic dust should be treated. For this multiscale simulation, the precise kinetic parameters, which can be estimated from the first-principle calculations, are required.

We have performed the first-principles calculations on the synthesis of the simplest amino acid, glycine, and methanol in interstellar environments in collaboration with the division of the astrophysics group. Nucleic acids and alkylphosphonic acids formations in the interstellar medium are the next targets. We will perform the first-principles calculations on the synthetic routes of them using the same protocol as analyzed for the glycine. We also explore the possibility of life using non-standard compounds such as Si-containing substances.

5) Development of Software

Due to the complexity and variety of life phenomena, different calculation methods and models have been used in the field of life science until now. In addition, it was difficult to calculate a sufficient time and size owing to the limitation in the current computer resources. In order to overcome the difficulty, it is necessary to develop new theories and methods with the help of collaboration among plural divisions and to conduct joint research on experiments and simulations. In this division, we have developed several methodologies for biomolecules in different levels.

For QM calculations, a GPU version of the fragment molecular orbital (FMO) method has been implemented. In order to use Cygnus, the mixed GPU and FPGA architecture, we will further implement GPU/FPGA version of OpenFMO. We also develop coupled cluster (CC)-type wave function methods in OpenFMO. For QM dynamics, the GPU version of the real-space density functional-based Car-Parrinello molecular dynamics simulation (we refer it as RS-CPMD) has been developed. However, the performance using the GPU architecture is not high enough. In collaboration with the division High-performance Computing System, we will enhance the performance of it on GPU architecture at first. For QM/MM calculations, QM(DFTB)/MM molecular dynamics (DFTB-MD) will be implemented for GPU/FPGA architecture too. For MD simulations, we will release python (or alternative ones) modules of PaCS-MD for the public. In order to evaluate the free energy landscape easily, modules of Global Reaction Route Mapping (GRRM) for free energy surface and analytic tools for metadynamics simulations will be developed.

5.5 Publications

Journal Papers

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4. T. Nakanishi, Y. Hori, H. Sato, S. Wu, A. Okazawa, N. Kojima, T. Yamamoto, Y. Einaga, S. Hayami, Y. Horie, H. Okajima, A. Sakamoto, Y. Shiota, K. Yoshizawa, O. Sato, "Observation of Proton Transfer Coupled Spin Transition and Trapping of Photoinduced Metastable Proton Transfer State in an Fe(II) Complex", *Journal of the American Chemical Society* **141**, 14384–14393 (2019). **DOI**:10.1021/jacs.9b07204
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8. T. Ohto, M. Dodia, J. Xu, S. Imoto, F. Tang, F. Zysk, T. D. Kühne, Y. Shigeta, M. Bonn, X. Wu, Y. Nagata, "Accessing the Accuracy of Density Functional Theory through Structure

and Dynamics of the Water–Air Interface", *The Journal of Physical Chemistry Letters* **10**(17), 4914-4919(2019). **DOI**:10.1021/acs.jpclett.9b01983

9. R. Harada, Y. Shigeta, "Selection Rules for Outliers in Outlier Flooding Method (OFLOOD) Regulate its Conformational Sampling Efficiency" to *Journal of Chemical Information and Modeling* **59**(12), 5198-5206 (2019). **DOI**:10.1021/acs.jcim.9b00
10. R. Harada, V. Sladek, Y. Shigeta, "Non-targeted Parallel Cascade Selection Molecular Dynamics Using Time-localised Prediction of Conformational Transitions in Protein Dynamics", *Journal of Chemical Theory and Computation* **15**, 5144-5153 (2019). **DOI**:10.1021/acs.jctc.9b00489
11. K. Kayanuma, M. Shoji, K. Furuya, K. Kamiya, Y. Aikawa, M. Umemura, Y. Shigeta, "First-principles study of the reaction mechanism of CHO + H on graphene surface", *The Journal of Physical Chemistry A* **123**, 5633-5639 (2019)
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5.6 Awards, Patent, and etc.

Awards

1. R. Harada, *Gakujyutsu-syo in 2019*, Molecular Simulation Society of Japan (Japan), (2019)
2. R. Harada, *13th Young Scientist Award*, Physical Society of Japan (Japan), (2019)
3. R. Harada, *67th Chemical Society of Japan Award for Young Chemists*, Chemical Society of Japan (Japan), (2018)
4. Y. Shigeta, *2018 Best Faculty Award*, University of Tsukuba (Japan), (2019).
5. Y. Shigeta, *22nd QSCP (Quantum Systems in Chemistry, Physics, and Biology) Promising Scientist Award*, Centre de Mécanique Ondulatoire Appliquée (France) (2017).
6. Y. Shigeta, *Outstanding Reviewers for Physical Chemistry Chemical Physics in 2016*, Royal Chemical Society (UK) (2017).
7. M. Kayanuma, *1st Chika Kuroda Award*, Ochanomizu University (Japan), (2016).
8. R. Harada, 1st Early Career Presentation Award, Biophysical Society of Japan (Japan), (2016).
9. M. Shoji, Daimon Prize, *3D active site, 2nd progress report conference* (Japan), (2015).

Patent

1. [**US Patent**] US 10,275,512 B2: Information Processing Apparatus and Index Dimension Extracting Method, T. Nakamura, R. Harada, Y. Shigeta
2. [**Domestic Patent**] Patent No. 6558754, Information Processing Apparatus and Index Dimension Extracting Method, T. Nakamura, R. Harada, Y. Shigeta

6 Division of Life Sciences: Molecular Evolution Group

6.1 Overview

Molecular Evolution Group in Division of Life Sciences has tackled unsolved problems in evolutionary biology. In particular, we are interested in the evolutionary process that has shaped extant molecular mechanisms and genomes in modern eukaryotic cells. During the period from 2014 to 2019, the following topics have been investigated.

Global eukaryotic phylogeny: We have no concrete vision regarding the relationship amongst major eukaryotic lineages, which were separated from one another in early eukaryotic evolution, as (i) phylogenetic 'signal' in the sequence data analyzed is insufficient, and (ii) the sequence data are available from only restricted members of eukaryotes. To overcome the first issue, "phylogenomic" analyses based on super-matrices of proteins, which typically comprise 50-300 genes identified in genome and/or transcriptome analyses, have been conducted these days. In theory, we can expect a greater amount of phylogenetic signal in multigene alignments than that in a single gene. Thus, phylogenomic analyses are anticipated to resolve ancient splits in the tree of eukaryotes with confidence. To counter the second issue, previously unstudied eukaryotes (novel eukaryotes) have been surveyed in natural environments. At the same time, there is a number of eukaryotes, of which phylogenetic positions remain unsettled (so-called "orphan" eukaryotes). Thus, to elucidate the ancient splits in the tree of eukaryotes, we believe that phylogenomic analyses of novel and/or orphan eukaryotes are indispensable.

Evolution of mitochondria: Diverse eukaryotes possess respiration organelles, mitochondria, which were derived from a single endosymbiosis of an α-proteobacterium. As the first mitochondrion was most likely established in the last common ancestor of eukaryotes, this endosymbiosis should have possessed a huge impact on early eukaryotic cell and genome evolutions. Because of the bacterial ancestry of mitochondria, the mitochondria in the vast majority of eukaryotes retain their own genomes. Nevertheless, the size, architecture, and gene content vary among the mitochondrial genomes, suggesting that mitochondrial genomes have been modified drastically during the evolution of eukaryotes. Furthermore, the species/lineages, which adapted to anaerobic/microaerophilic environments, possess structurally and functionally reduced mitochondria (mitochondrion-related organelles or MROs). MROs emerged multiple branches in the tree of eukaryotes, but the metabolic capacities in the extant MROs are similar to each other. Thus, some evolutionary constraints may exist in the process of adapting to anaerobic/microaerophilic environments, albeit we have yet to understand the process mentioned above.

Evolution of plastids: Plastids in photosynthetic eukaryotes were originated from a single endosymbiotic cyanobacterium in the common ancestor of Archaeplatida comprising glaucophytes, red algae, and green plants (green algae plus land plants). In the later evolution, plastids further spread into multiple eukaryotic lineages through multiple endosymbioses of green/red alga in distantly related heterotrophic eukaryotes. We designate the cyanobacterial endosymbiosis in the ancestral archaepalstid species as primary endosymbiosis and the endosymbioses between green/red algae and heterotrophic eukaryotes as secondary endosymbioses. Although both primary and secondary endosymbioses are significant for understanding the diversity and evolution of eukaryotes, the detailed process transforming an endosymbiont into an organelle (plastid) has yet to be understood.

Evolution of bacterial endosymbionts in diverse eukaryotic cells: The evolutionary processes, which transformed an α-proteobacterium into the ancestral mitochondrion and a cyanobacterium into the ancestral plastid, are difficult to retrace, as the key information to infer these ancient events has already been lost in the latter evolution. To overcome the difficulty in studying the endosymbiosis-driven processes generating the mitochondrion and plastid, eukaryotes with bacterial endosymbionts, which reside in but have not fully integrated into the host (eukaryotic) cells, have been anticipated to retain intermediate traits of the transition of a bacterial endosymbiont into an organelle.

Studies based on the collaboration with other divisions/groups in the institute: We have collaborated with Database Group in the Division of Computational Informatics to develop a program analyzing amino acid sequences to predict whether a protein can be localized in the mitochondrion/MRO. Another intra-institutional collaboration has been developed with Biological Function and Information Group. In this collaboration, we combined molecular phylogeny and quantitative simulations of protein tertiary structures to evaluate the proposed function of a protein family of which experimental information has not been accumulated.

6.2 Research Results

1) Global eukaryotic phylogeny

Proposal for a new super-group of eukaryotes

Recent phylogenomic analyses typically show a eukaryote tree consisting of four major assemblages: (1) Amorphea (Amoebozoa plus Obazoa, the latter including animals and fungi), (2) Diaphoretickes (primarily SAR, Archaeplastida, Cryptista, and Haptoptista), (3) Discoba, and (4) Metamonada. Nonetheless, there are several "orphan" eukaryotes that cannot be assigned to any assemblage by cellular morphology (including ultrastructural characteristics) or single-gene phylogenies (typically inferred from small subunit ribosomal RNA genes). Prior to this study, phylogenetic/phylogenomic analyses including *Collodictyon triciliatum*, *Mantamonas plastica*, and *Rigifila ramosa* failed to place in or branch with any of the four assemblages, implying that their phylogenetic positions may be significant for our understanding of deep eukaryote history. Unfortunately, the phylogenetic positions of *Collodictyon*, *Mantamonas*, and ancyromonads remained unclear, likely due to the phylogenetic signal in the previously analyzed sequence data being insufficient. Therefore, we undertook phylogenomic analyses that incorporated deeply sequenced transcriptome data from two collodictyonids (*Collodictyon triciliatum* and *Diphylleia rotana*), *Mantamonas plastica*, and *Rigifila ramosa* (Figs. 1A-D).

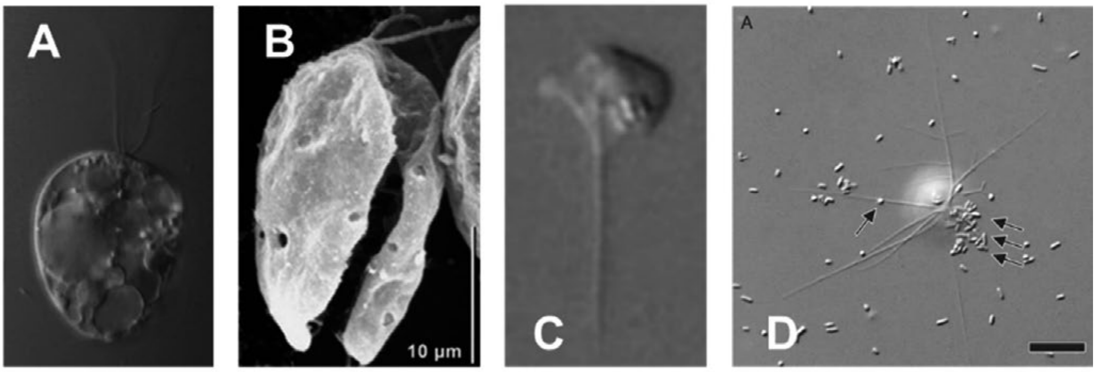

Figure 1. "Orphan" eukaryotes examined in this study. **A.** *Collodictyon triciliatum* (https://www.apollon.uio.no/english/articles/2012/microorganism.html), **B.** *Diphylleia rotana*. (http://tolweb.org/Protists_of_uncertain_placement/2383), **C.** *Mantamonas plastica*, (Glucksman et al. 2011 ***Protist***), and **D.** *Rigifila ramosa* (Yabuki et al. 2013 ***Protist***).

The phylogenetic analyses based on a super-matrix including 351 proteins (97,002 amino acid positions in total) recovered a robustly supported clade comprising collodictyonids, *Rigifila*, and *Mantamonas* (Fig. 2). Overall, the 351-protein phylogeny suggests that collodictyonids, *Rigifila*, and *Mantamonas* form a major eukaryote clade that has been overlooked in previously published studies. No name exists for this putative super-group, and it is obviously premature to propose a formal taxon. We suggested the place-holding moniker "CRuMs" (collodictyonids, *Rigifila*, *Mantamonas*), which is euphonic and evokes the species-poor nature of these taxa.

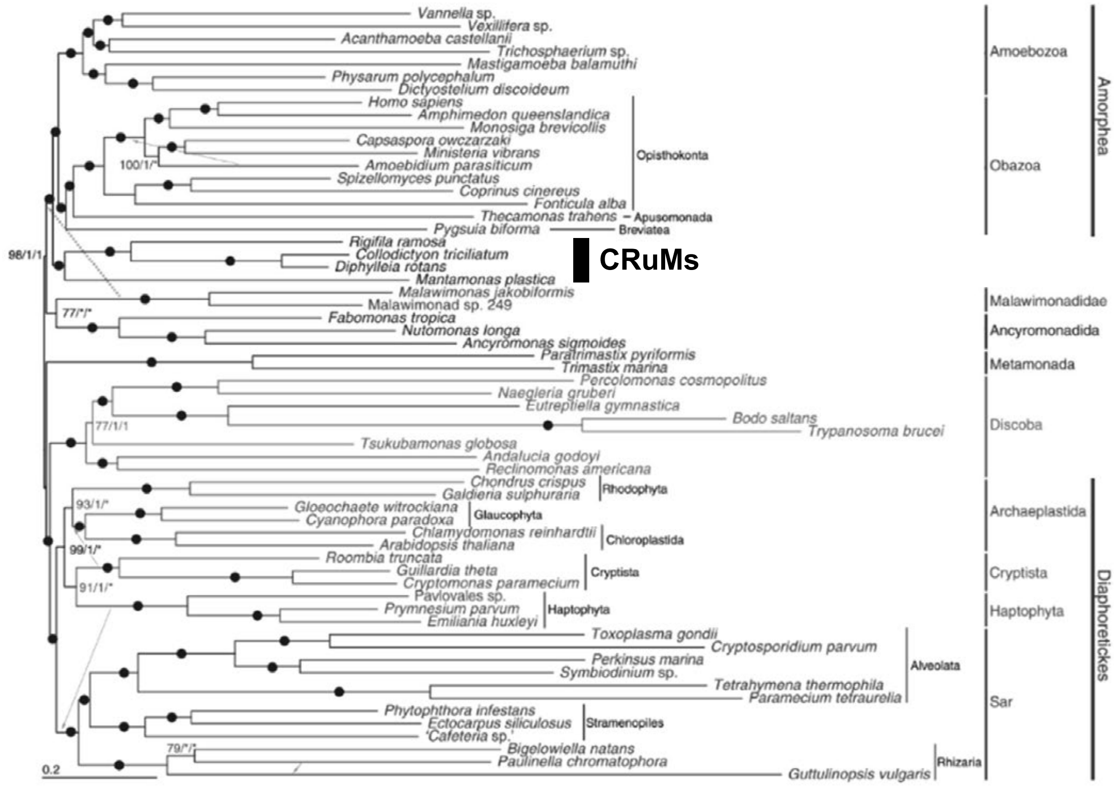

Figure 2. Maximum Likelihood Phylogenetic tree for 61 eukaryotes, inferred from 351 proteins under the LG + C60 + F + Γ-PMSF model. The numbers on branches show ML bootstrap support values from 100 replicates. Filled circles represent the fully supported nodes in the bootstrap analysis. The original figure was presented in ***Genome Biol Evol*** 2018 10:427–433 as Fig. 1.

This work was an international joint research among groups in the US, Canada, and Japan, and was published in ***Genome Biol Evol*** (2018 10:427–433; this article has been cited 36 times as of January 2020). Furthermore, our unpublished phylogenomic analyses placed (1) an orphan eukaryote called *Glissandra* (strain SRT312) and (2) a previously undescribed eukaryote strain SRT605 within the CRuMs clade, suggesting that we still underestimate the diversity of "CRuMs".

The tree of Fornicata and evolution of the function of MROs

Many anaerobic microbial parasites possess highly modified mitochondria known as mitochondrion-related organelles (MROs). The best-studied of these are the hydrogenosomes of *Trichomonas vaginalis* and *Spironucleus salmonicida*, which produce ATP anaerobically through substrate-level phosphorylation with concomitant hydrogen production; and the mitosomes of *Giardia intestinalis*, which are functionally reduced and lack any role in ATP production. However, to understand the metabolic specializations that these MROs underwent in adaptation to parasitism, data from their free-living relatives are needed. We conducted a large-scale comparative transcriptomic study of free-living members of a major eukaryotic group, Metamonada. Based on the deeply sequenced transcriptome data, we prepared a super-matrix comprising 159 proteins and examined the phylogenetic relationship among metamonads. The sequence data were used also for estimating lineage-specific gain and loss of metabolic functions in the metamonad MROs.

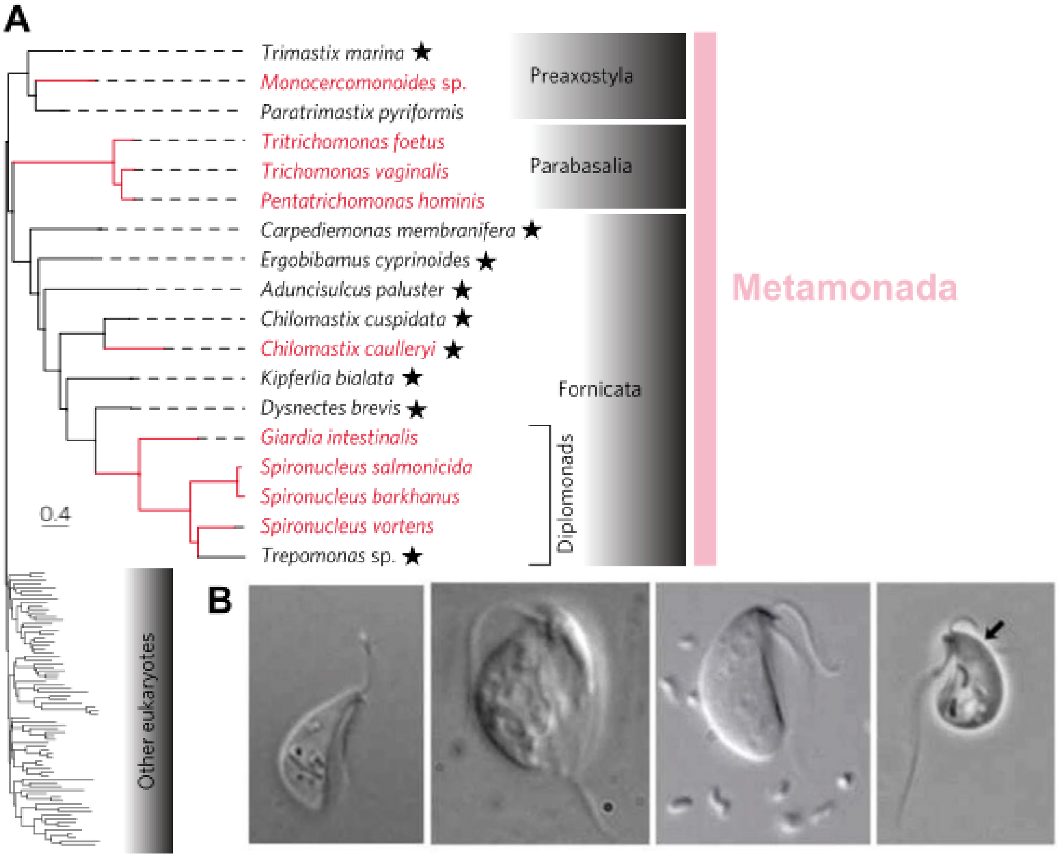

Figure 3. (A) Maximum Likelihood phylogenetic tree for 18 metamonads and 76 other eukaryotes, inferred from 159-protein super-matrix under the LG + Γ + F model. All of the bipartitions in the Metamonada clade received full ML bootstrap supports (not shown). Parasitic species are shown in red. We generated transcriptome data from the species marked by stars. Filled circles represent the fully supported nodes in the bootstrap analysis. The original figure was presented in ***Nat Ecol Evol*** 2017 1:0092 as Fig. 1. (B) Four typical free-living metamonads studied in this work. From left to right, *Dysnectes brevis*, *Aduncisulcus paluster*, *Kipferlia bialata*, and *Ergobibamus cyprinoides*. Images were taken from ***Nat Ecol Evol*** website (https://natureecoevocommunity.nature.com/users/34134-andrew-j-roger/posts/15190-endless-forms-most-wonderful-new-forms-of-mitochondria-in-free-living-microbial-eukaryotes).

The ML tree inferred from a 159-protein super-matrix (39,089 amino acid positions in total) robustly resolved the relationship among the members of Metamonada (Fig. 3A). We also analyzed the transcriptomic data to predict proteins localized in the MRO for each metamonad species. By mapping the predicted metabolic capacities on the highly resolved tree of Metamonada, we successfully uncovered a complex history of ATP production machinery in diplomonads (e.g., *Giardia*) and their closest free-living relative, *Dysnectes*, and a correlation between the glycine cleavage machinery and lifestyles.

This work was an international joint research among groups in the US, Sweden, Czech Republic, Japan, and Canada, and published in ***Nat Ecol Evol*** (2017 1:0092; this article has been cited 30 times as of January 2020). Related to the publication of this article, ***Nat Ecol Evol*** published a commentary by Dr. Andrew J. Roger

(see https://natureecoevocommunity.nature.com/users/34134-andrew-j-roger/posts/15190-endless-forms-most-wonderful-new-forms-of-mitochondria-in-free-living-microbial-eukaryotes). ***Nature Japan*** also published an interview on three principle authors in Japan (Drs. Tetsuo Hashimoto and Yuji Inagaki in Univ. Tsukuba, and Ryoma Kamikawa in Kyoto Univ; see https://www.natureasia.com/ja-jp/natecolevol/interview/contents/4). To pursue the unique metabolic properties in the MROs of free-living metamonads further, we sequenced and published the draft genome of *Kipferlia bialata* (the third image in Fig. 3B) in ***PLOS One*** (2018 13: e0194487). We are currently sequencing the genomes of *Dysnectes* and *Aduncisulcus* (the first and second images in Fig. 3B).

Other phylogenomic studies

Besides the two works described above, we published three phylogenomic works (see below). Firstly, the relationship among the five orders in the class Kinetoplastea was examined and robustly resolved by phylogenetic analyses of a 43-protein super-matrix (Yazaki et al. ***Genes Genet Syst*** 2017 92:35-42). Secondly, our phylogenomic analyses of a 75-protein super-matrix indicated the independent emergences of green alga-derived, non-canonical plastids in the evolution of dinoflagellates with confidence (Sarai et al. ***Proc Nat Acad Sci USA*** 2020 in press). Finally, we successfully pinpointed the phylogenetic position of an orphan lineage, barthelonids, by analyzing a 153-protein super-matrix (Yazaki et al. 2019 ***bioRχiv***; doi: 10.1101/805762).

2) Evolution of mitochondria

Since 2014, we completely sequenced and published the mitochondrial genomes of five eukaryotes: Two members belonging to Haptista (*Chrysochromulina* sp. and *Marphrys* sp.) and three members belonging to Cryptista (*Palpitomonas bilix*, *Leucocryptos marina*, and *Hemiarma marina*).

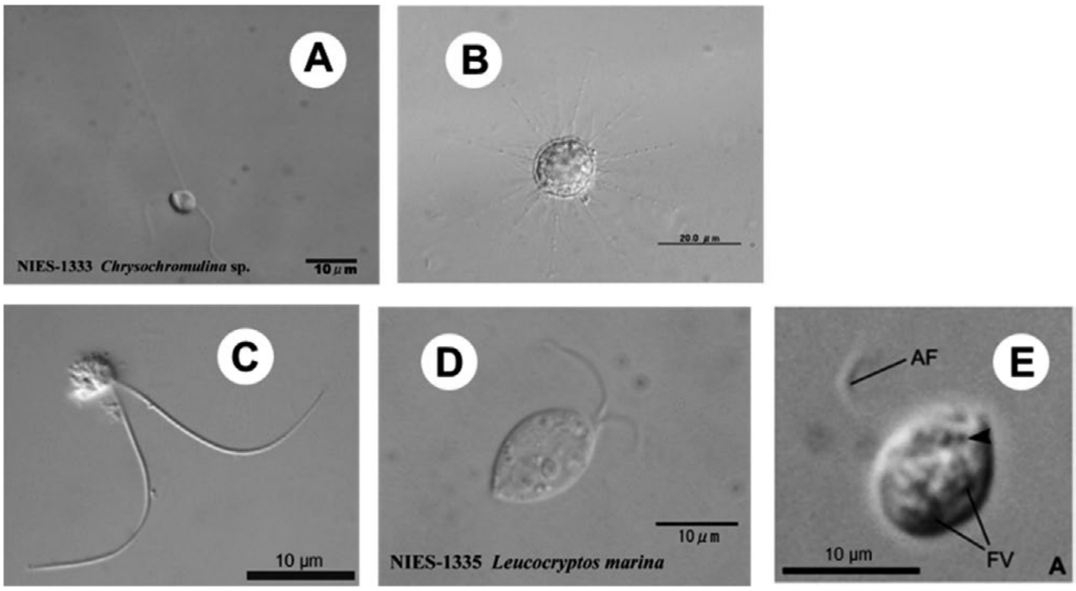

Figure 4. Eukaryotes of which mitochondrial genomes were completely sequenced. (A) *Chrysochromulina* sp. NIES 1333 (https://shigen.nig.ac.jp/algae/images/strainsimage/nies-1333.jpg), (B) *Marophrys* sp. SRT127 (Fukuda & Ishida 2014 ***Tsukuba J Biol*** 13), (C) *Palpitomonas bilix* (Yabuki et al. 2010 ***Protist*** 161:523-538), (D) *Leucocryptos marina* (https://shigen.nig.ac.jp/algae/images/strainsimage/nies-1335.jpg), (E) *Hemiarma marina* (Shiratori & Ishida 2016 ***J Eukaryot Microbiol*** 63:804–812).

Mitochondrial genomes of two haptists

Recent phylogenomic studies grouped haptophytes and centrohelids into a phylogenetic assemblage “Haptista”. We sequenced and published the mitochondrial genomes of a haptophyte *Chrysochromulina* sp. NIES 1333 and a centrohelid *Marophrys* sp. SRT127 in ***Mobile Genet Elements*** (2014 4:e29384) and ***Sci Rep*** (2019 9:4850), respectively.

Mitochondrial genomes of three cryptists

Cryptophytes, a taxonomic group of photosynthetic eukaryotes, appeared to be closely related to multiple heterotrophic lineages/species, goniomonads, kathablepharids, *Hemiarma marina*, and *Palpitomonas bilix*, forming a phylogenetic assemblage “Cryptista”. We have been interested in the mitochondrial genome evolution in Cryptista and completely sequenced the mitochondrial genomes of a kathablepharid *Leucocryptos marina*, *Hemiarma*, and *Palpitomonas*. The *Palpitomonas* mitochondrial genome was found to be a single linear molecule comprising “single copy region” (~16 Kb) and repeat regions (~30 Kb) arranged in an inverse manner at both ends of the genome (~62 Kb in total). Linear mitochondrial genomes with large inverted repeats are known for three distantly related eukaryotes (including *Palpitomonas*), suggesting that this unique genome structure has emerged at least three times in the entire mitochondrial evolution. This work was published in ***Genome Biol Evol*** (2016 8:3090–3098). We recently sequenced the mitochondrial genomes of two members of Cryptista, *Leucocryptos* and *Hemiarma* (Fig. 5).

Combined the two newly sequenced mitochondrial genomes with those of other cryptists, we proposed the scenarios for the evolution of cytochrome *c* maturation in the Cryptista clade (Currently reviewed to be published in ***Front Ecol Evol***). This work is a joint research with Drs. Yuki Nishimura and Moriya Ohkuma in RIKEN BioResource Research Center, Japan and Dr. Keitaro Kume in Faculty of Medicine, University of Tsukuba, Japan.

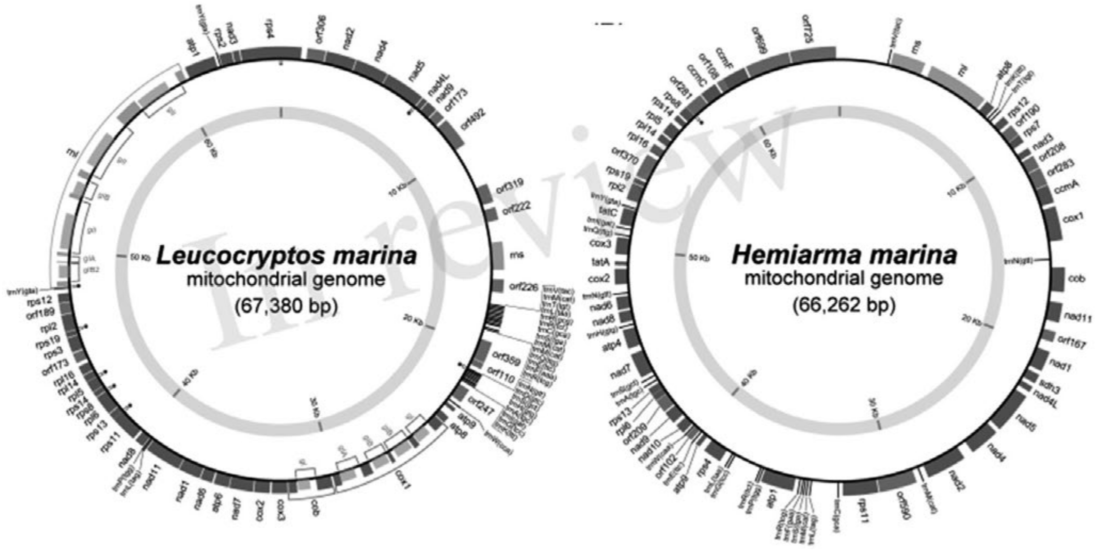

Figure 5. Mitochondrial genomes of *Leucocryptos marina* (left) and *Hemiarma marina* (right). Gene coding regions and transfer RNA genes are shown in boxes and lines, respectively.

3) Evolution of plastids

Plastid genome evolution triggered by secondary loss of photosynthesis

Loss of photosynthesis is a recurring theme in eukaryotic evolution. In organisms that have lost the ability of photosynthesis, non-photosynthetic plastids are retained because they play essential roles in processes other than photosynthesis. The genomes of secondarily non-photosynthetic plastids tend to be more reduced than those of photosynthetic plastids in terms of both genome size and gene repertory. To retrace the reductive process worked on non-photosynthetic plastid genomes, we sequenced and analyzed the plastid genomes of non-photosynthetic species in two algal groups, cryptophytes and diatoms (Tanifuji et al. 2020 ***Genome Biol Evol*** in press; Kamikawa et al. 2015 ***Mol Biol Evol*** 7:1133-1140).

In Tanifuji et al. (2020), we newly sequenced the plastid genomes of two non-photosynthetic species and one photosynthetic species, and revealed that distinct sets of photosynthesis-related genes were lost from the plastid genomes of multiple cryptophytes that lost photosynthesis separately. Kamikawa et al. (2015) sequenced the plastid genome of a non-photosynthetic diatom *Nizschia* sp. NIES-3581 and proposed a functional constraint against the loss of ATP synthase genes from non-photosynthetic plastid genomes. The two works described above are joint researches with Dr. Goro Tanifuji in National Museum of Nature and Science, Japan, and Dr. Ryoma Kamikawa in Kyoto University, Japan.

Origins of green-colored plastids in dinoflagellates inferred from plastid genome-based phylogenies

An assemblage of eukaryotic algae, dinoflagellates, is unique in plastid evolution. The ancestral dinoflagellate cell is believed to have a plastid containing a characteristic pigment called peridinin, and this “peridinin plastid” has been inherited to the vast majority of the extant photosynthetic descendants. Nevertheless, multiple dinoflagellate lineages are believed to have replaced the original plastid containing peridinin through endosymbioses of diverse algae. A dinoflagellate *Lepidodinium chlorophorum* possesses a green-colored plastid containing chlorophylls *a* and *b*, albeit we were unsure which algal gave rise to the current plastid in this dinoflagellate. We sequenced the plastid genome of *Lepidodinium* and prepared a super-matrix containing 52 proteins that are encoded in the plastid genome. Phylogenetic analyses of 52-protein super-matrix robustly showed an intimate affinity between the plastid of *Pedinomonas minor*, which is a member of a small green algal group Peidnophyceae, and that of *Lepidodinium*. Thus, we concluded the ancestral *Lepidodinium* engulfed an alga belonging to Pedinophyceae, followed by the transformation of the endosymbiont alga into the current green-colored plastid. These results were published in ***Genome Biol Evol*** (2015 7:1133-1140).

We currently collaborate with Drs. Takahashi and Iwataki in the University of Tokyo, Japan, to explore the diversity of dinoflagellates with green-colored plastids. So far, two dinoflagellate strains with green-colored plastids have been identified (TRD-132 and MRD-151; Sarai et al. ***Proc Nat Acad Sci USA*** 2020 in press). To elucidate the origins of the green-colored plastids of strains TRD-132 and MRD-151, we sequenced their plastid genomes (the left and center images in Fig. 6; Matsuo et al. unpublished results) and conducted a plastid genome-based phylogenetic analysis as done in Kamikawa et al. (2015). In the plastid genome-based phylogeny (based on 51 plastid-encoded proteins), *Lepidodinium*, TRD-132, and MRD-151 grouped together and connected to pedinophyte green algae with high statistical support (the right image in Fig. 6; Matsuo et al. unpublished results). Thus, we concluded that the same pedinophyte green alga (or closely related pedinophyte green algae) is the origin(s) of the green-colored plastids of *Lepidodinium*, TRD-132, and MRD-151.

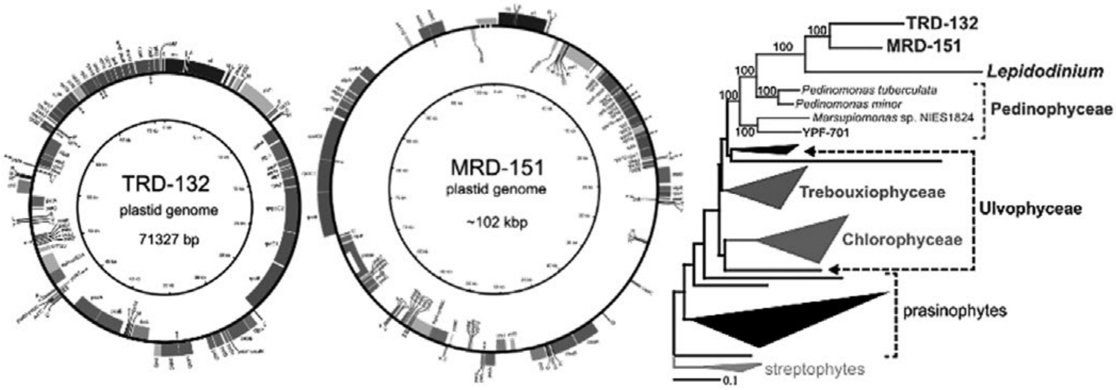

Figure 6. Plastid genomes of dinoflagellate strains TRD-132 (left) and MRD-151 (center). Gene coding regions and transfer RNA genes are shown in boxes and lines, respectively. The plastid genome-based phylogeny (right) robustly grouped the three green dinoflagellates (TRD-132, MRD-151, and *Lepidodinium*) and members of Pedinophyceae together.

4) Evolution of bacterial endosymbionts in diverse eukaryotic cells

Cyanobacterial endosymbionts in rhopalodiacean diatoms

The evolution of mitochondria and plastids from bacterial endosymbionts were key events in the origin and diversification of eukaryotic cells. Although the ancient nature of these organelles makes it difficult to understand the earliest events that led to their establishment, the studies of eukaryotic cells with recently evolved obligate endosymbiotic bacteria have the potential to provide important insights into the transformation of endosymbionts into organelles. Diatoms belonging to the family Rhopalodiaceae and their endosymbionts of cyanobacterial origin (i.e., “spheroid bodies”) are emerging as a useful model system in this regard. The spheroid bodies, which appear to enable rhopalodiacean diatoms to use gaseous nitrogen, became established after the divergence of extant diatom families. We sequenced the first and second complete genome sequences of spheroid bodies in two rhopalodiacean diatoms *Epithemia turgida* and *Rhopalodia gibberula*. Both spheroid body genomes possess a gene set for nitrogen fixation, but has lost photosynthetic ability indicating that the spheroid bodies are metabolically dependent on their host cells. A severe reductive pressure most likely worked on the spheroid body genomes, as the genomes appeared to be reduced in both size and gene repertory. We proposed that the diatom-spheroid body endosymbiosis is thus a unique system for investigating the processes underlying the integration of a bacterial endosymbiont into eukaryotic cells. The spheroid body genomes of *Epithemia* and *Rhopalodia* were published in ***Proc Nat Acad Sci USA*** (2014 111:11407-11412) and ***Sci rep*** (2017 7:13075), respectively, and the former article has been cited 71 times as of December 2019. After the publication of the first article of the spheroid body genome, Drs. Nakayama and Inagaki were invited to publish a review article on this particular topic in ***Acta Soc Bot Pol*** (2014 83:409-41).

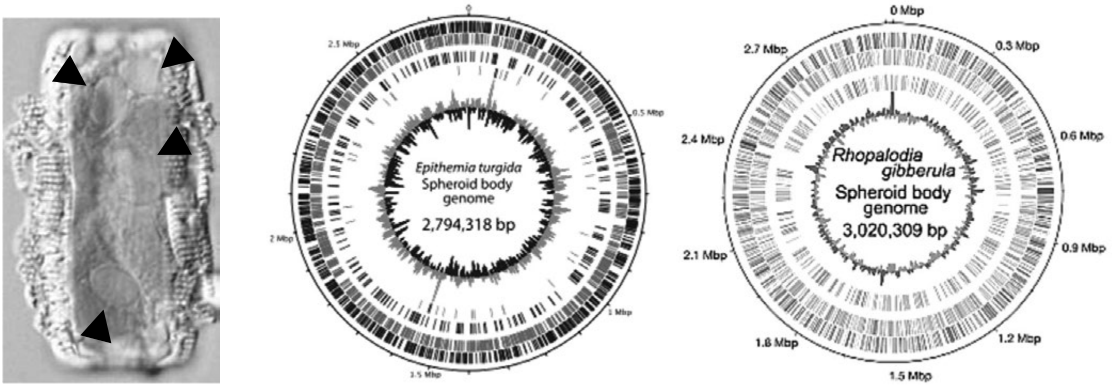

Figure 7. Left, a rhopalodiacean diatom. Spheroid bodies are highlighted by arrowheads. This image was taken by Dr. Nakayama (Tohoku Univ.). Center, a circular genome map of the spheroid body genome of *Epithemia turgida* (Nakayama et al. 2014). Right, a circular genome map of the spheroid body genome of *Rhopalodia gibberula* (Nakayama et al. 2017).

A cyanobacterial symbiont associated with a dinoflagellate *Ornithocercus magnificus*

Besides the cyanobacterial endosymbionts in rhopalodiacean diatoms (spheroid bodies), we are greatly interested in the origin and function of diverse bacterial symbionts in/associated with eukaryotes. We sequenced the genome of cyanobacteria collected from a cell of a pelagic dinoflagellate (*Ornithocercus magnificus*) that is known to host cyanobacterial symbionts (OmCyn) within a specialized chamber (Fig. 8, left). Phylogenetic analyses using the OmCyn genome sequence revealed that the cyanobacterium represents an under-described lineage within an extensively studied, ecologically important group of marine cyanobacteria (Fig. 8, center). The protein repertory encoded in the OmCyn genome appeared to be reduced compared to its free-living relatives (Fig. 8, right), suggesting that the OmCyn genome has been reduced due to the symbiotic lifestyle. Metagenomic analyses demonstrated that this cyanobacterial lineage is globally distributed and strictly coexists with its host dinoflagellates, suggesting that the intimate symbiotic association allowed the cyanobacterium to escape from previous metagenomic studies. Discovery of this cyanobacterial lineage, hidden by its symbiotic lifestyle, provides crucial insights into the diversity, ecology, and evolution of marine cyanobacteria and suggests the existence of other undiscovered cryptic cyanobacterial lineages. This work was published in ***Proc Nat Acad Sci USA*** (2019 116:15973-15978). In this same issue, the image of the dinoflagellate cell that investigated was selected as the journal cover, and a commentary on our work was published (Archibald, ***Proc Nat Acad Sci USA*** 2019 116:15757-15759).

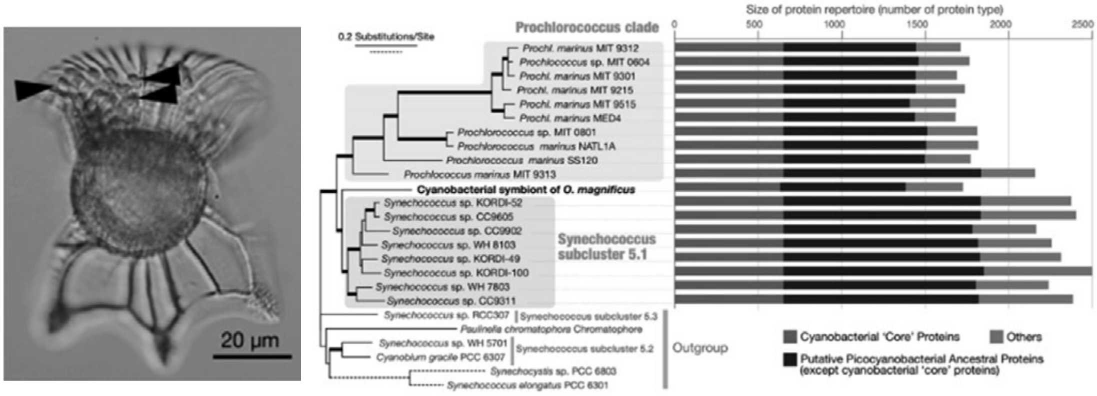

Figure 8. Left, *Ornithocercus magnificus*. The cyanobacterial symbionts are highlighted by arrowheads. Center, the ML phylogenetic analyses based on 41 proteins shared among cyanobacteria. The cyanobacterial symbiont of *Ornithocercus* (OmCyn) shows no clear affinity to any of the known marine picocyanobacteria. Right, Comparison of protein numbers among marine picocyanobacteria. OmCyn seemingly possesses a smaller-size proteome than its free-living relatives, suggesting that the OmCyn genome has been reduced during the symbiotic lifestyle. All images are taken from Nakayama et al. (2019) and modified.

5) Studies based on the collaboration with other divisions/groups in Center for Computational Sciences, University of Tsukuba

Estimation of the interactions between tRNA and translation factors

Translation elongation factor-1α (EF-1α) or its paralog elongation factor-like proteins (EFL) interact with an aminoacyl-transfer RNA (aa-tRNA) to play its essential role in elongation of peptide-chain during protein synthesis. Eukaryotic species usually have either an EF-1α or EFL protein; however, some species have both EF-1α and EFL (dual-EF-containing species). In the dual-EF-containing species, EF-1α appeared to be highly divergent at the primary structural level. Homology modeling and surface analysis of EF-1α and EFL were performed to examine the hypothesis that the divergent EF-1α in the dual-EF-containing eukaryotes does not strongly interact with aa-tRNA compared to the canonical EF-1α and EFL. The subsequent molecular dynamics simulations were carried out to confirm the validity of modeled structures and to analyze their stability. We found that the molecular surfaces of the divergent EF-1α proteins were negatively charged partly, and thus they might not interact with negatively charged aa-tRNA as strongly as the canonical ones (Fig. 9). This work was a joint research with Drs. Megumi Kayanuma and Yasuteru Shigeta in Biological Function and Information Group (Division of Life Sciences), and published in ***ACS Omega*** (2019 4:7308-7316).

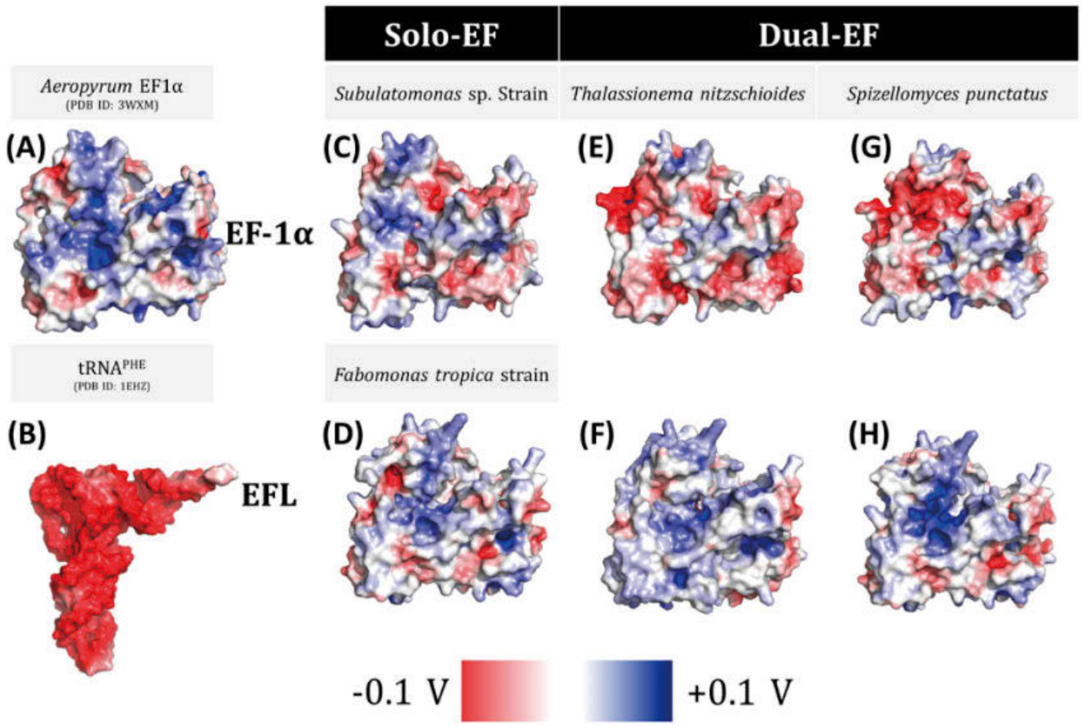

Figure 9. Surface electrostatic distribution of the template protein aa-tRNA and EF-1α/EFL models, generated using the SWISS-MODEL using an archeon *Aeropyrum permix* EF-1α (PDB ID: 3WXM) as the template, obtained using the eF-surf web server.

Development of a software predicting mitochondrion-localized proteins

To estimate the metabolic functions of mitochondria in diverse eukaryotes, the mitochondrial proteomes are useful. However, the mitochondrial proteomes are currently restricted to major organisms in biology (i.e., model organisms). For nonmodel organisms, recent advances in sequence technology allow us to generate transcriptome/genome sequence data, followed by *in silico* prediction of mitochondrion-localized (mt-localized) proteins based on the corresponding sequence data. So far, various prediction methods that are trained using the proteins of model organisms belonging particularly to animals, plants, and fungi exist. However, such methods may not be suitable for predicting the proteins derived from nonmodel organisms because the sequence features of the mt-localized proteins of diversified nonmodel organisms can differ from those of model organisms. We proposed NommPred, which predicts the mt-localized proteins of nonmodel organisms that are widely distributed over eukaryotes. We used a gradient boosting machine to develop two predictors—one for predicting the proteins of mitochondria and the other for predicting the proteins of mitochondrion-related organelles that are highly reduced mitochondria. The performance of both predictors was found to be better than that of the best method available. This work was a joint research with Drs. Toshiyuki Amagasa and Hiroyuki Kitagawa in Database Group (Division of Computational Informatics), and published in ***Evol Bioinformat*** (2018 14:1-12). The software developed in this study (NommPred) is distributed in GitLab (https://gitlab.com/kkei/NommPred.git).

Re-evaluation of the tertiary structure of CysN

Diverse bacteria possess ATP sulfurylase that produces adenosine-5′-phosphosulfate from ATP and sulfate, coupled with GTP hydrolysis. This enzyme composes of small and large subunits (CysC and CysN) and the latter has been known to bear the amino acid sequence similarity to EF-Tu, a highly conserved protein involved in translation elongation in bacteria. EF-1α in eukaryotes and archaea is homologous to EF-Tu, and the N-terminal domain of EF-1α contains an α-helix that is absent for EF-Tu. Interestingly, although CysN and EF-Tu are both bacterial proteins, CysN showed a closer phylogenetic affinity to EF-1α than EF-Tu. If the phylogenetic affinity between EF-1α and CysN is genuine, CysN may possess the EF-1α-specific α-helix in the N-terminal domain. The tertiary structure of CysN was resolved in 2006. Unfortunately, the crystal lacks the region that corresponds to the EF-1α-specific α-helix and the similarity between CysN and EF-1α at the structural level could not be examined. Thus, we predicted the tertiary structure of the N-terminal portion of CysN by a 2 μs all-atom molecular dynamics simulation in explicit water. As shown in Fig. 10, CysN was predicted to bear an α-helix, which is likely homologous to the helix only found in EF-1α, in the N-terminal domain. Our *in silico* prediction of the CysN tertiary structure favors the EF-1α origin of CysN. This study is a joint research with Dr. Ryohei Harada in Biological Function and Information Group (Division of Life Sciences). The manuscript on this matter is currently under preparation.

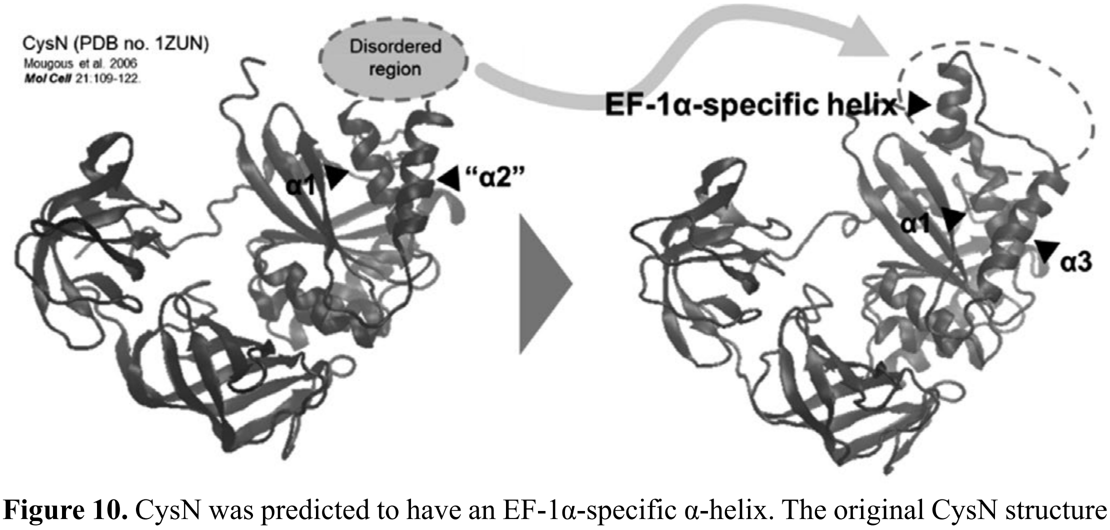

Figure 10. CysN was predicted to have an EF-1α-specific α-helix. The original CysN structure (left) contains a disordered region in the N-terminal domain. The disordered region in the original CysN structure was predicted to form an α-helix, which is absent in the bacterial homolog (i.e. EF-Tu) but likely homologous to α2 in EF-1α

6.3 Collaboration

Intra-institutional collaboration

We have collaborated with Drs. Yasuteru Shigeta and Ryhei Harada in Biological Function and Information Group to conduct studies combining phylogenetic and structural information on proteins (see 6.2.5). We co-supervised a graduate student (Keitaro Kume) with Drs. Toshiyuki Amagasa and Hiroyuki Kitagawa in Database Group as a part of the dual degree program between Graduate School of Life and Environmental Sciences and Graduate School of Systems and Information Engineering. This collaboration resulted in the development of computer software that can predict mitochondrion-localized proteins based on sequence data (see 6.2.5).

Domestic collaboration

We have investigated diverse eukaryotes, which are anticipated to provide key aspects in the global phylogeny of eukaryotes and/or evolutions of mitochondria, plastids, and bacterial endosymbionts (see 6.2.1.4). In these works, the collaboration with Drs. Akinori Yabuki and Takashi Shiratori (Japan Agency for Marine-Earth Science and Technology), Dr. Ken-ichiro Ishida (University of Tsukuba), Drs. Mitsunori Iwataki and Kazuya Takahashi (the University of Tokyo), and Dr. Yurika Ujiié (Kochi University) were crucial. In addition, we worked with members who left our group, such as Drs. Ryoma Kamikawa (University of Kyoto), Goro Tanifuji (National Museum of Nature and Science), Takuro Nakayama (Tohoku University), Yuki Nishimura (RIKEN), Euki Yazaki (the University of Tokyo), and Keitaro Kume (Faculty of Medicine, University of Tsukuba).

International collaboration

We conducted joint research projects with Drs. Andrew J. Roger, Alastair G. B. Simpson, and John M. Archibald, members of the Centre for Comparative Genomics and Evolutionary Bioinformatics in Dalhousie University, Canada. The collaboration with Drs. Roger and Simpson resulted in the two major topics described in section 6.2.1, and the ones with Dr. Archibald resulted in the topics related to the evolutions of plastids (section 6.2.3) and bacterial endosymbionts (section 6.2.4).

Besides the collaborations described above, we have worked together with Drs. Marek Eliáš (University of Ostrava, Czech Republic), Vladimír Hampl (Charles University in Prague, Czech Republic), Ensoo Kim (American Museum of National History, USA), Fabrizio Frontalini (Università degli Studi di Urbino "Carlo Bo", Italy), and Colomban De Vargas (CNRS and Station Biologique de Roscoff, France). Some results from the joint researches with the above collaborators have been published in a peer-reviewed journal (Záhonová et al.

2018 ***Sci Rep*** 8:5239; Ciacci et al. 2019. ***Sci Rep*** 19:19441).

6.4 Future Plan

We continue challenging to resolve the global eukaryotic phylogeny by subjecting eukaryotes, which may hold keys to understand questions in the cellular and genome evolutions in eukaryotes, to phylogenomic analyses. We will begin with orphan eukaryotes *Microheliella maris* and *Glissandria* sp., and previously undescribed eukaryotes strain SRT308, SRT605, and SRT706, as we have already generated their transcriptome data and prepared super-matrices.

We will conduct mitochondrial genome sequencing analyses on the eukaryotes of which phylogenetic positions are anticipated to be significant in terms of the evolution of mitochondria. For instance, our preliminary phylogenomic analysis of SRT308 suggested that this eukaryote occupies the ancestral position of Euglenozoa of which members are known to be unique in mitochondrial genome structure. Thus, the mitochondrial genome of SRT308 may provide clues to understand how euglenozoans shaped their unique mitochondrial genomes. We are also interested in the mitochondrial genomes of foraminifers and radiolarians, as no mitochondrial genome is available for these eukaryotes.

We are interested in dinoflagellates bearing non-canonical plastids that were derived from diverse endosymbiotic algae. To pinpoint the origins of non-canonical dinoflagellate plastids, phylogenetic analyses based on plastid genome data are useful. Thus, we will sequence the genomes of non-canonical dinoflagellate plastids. For instance, the genome of a non-canonical plastid containing chlorophylls *a* and *b* in *Oxytoxum* sp. strain SG-436 will be the first target.

The projects on sequencing bacterial endosymbionts will be continued. We have already started sequencing the genome of the cyanobacterial endosymbiont in a diatom *Epithemia adnata* and bacterial endosymbionts in dinoflagellate *Histioneis depressa*. In addition, we are working on sequencing the bacterial endosymbionts in a foraminifer *Ammonia beccarii*.

Finally, we will continue collaborating with Biological Function and Information Group (Division of Life Sciences) in Center for Computational Sciences to conduct joint researches on the evolution of proteins by combining the phylogenetic and structural information. We recently started working on a project on the evolution of a protein involved in translation termination in eukaryotes and archaea. After finishing the above project, we plan to assess the evolution of EF-1α in microsporidia and a protein involved in autophagy by combining the phylogenetic and structural information.

6.5 Publications

Journal Papers (refereed)

1. C. Sarai, G. Tanifuji, T. Nakayama, R. Kamikawa, K Takahashi, H. Miyashita, K. Ishida, M. Iwataki & Y. Inagaki, *Proceedings of the National Academy of Sciences of the United States of America*, vol. 117, 5364-5375 (2020)
2. G. Tanifuji, R. Kamikawa, C. E. Moore, T. Mills, N. T. Onodera, Y. Kashiyama, J. M. Archibald, Y. Inagaki & T. Hashimoto, *Genome Biology and Evolution,* vol. 12, 3926-3937. (2020)
3. C. Ciacci, M. V. Grimmelpont, I. Corsi, E. Bergami, D. Curzi, D. Burini, V. M. P. Bouchet, P. Ambrogini, P. Gobbi, Y. Ujiié, Y. Ishitani, R. Coccioni, J. M. Bernhard & F. Frontalini, *Scientific Reports*, vol. 19, 19441 (2019)
4. I. Yuyama & T. Higuchi, *PeerJ*, vol. 7, e7241 (2019)
5. T. Nakayama, M. Nomura, Y. Takano, G. Tanifuji, K. Shiba, K. Inaba, Y. Inagaki & M. Kawata, *Proceedings of the National Academy of Sciences of the United States of America*, vol. 116, 15973-15978 (2019)
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7. K. Sakamoto, M. Kayanuma, Y. Inagaki, T. Hashimoto, Y. Shigeta, *ACS Omega*, vol. 4, 7308-7316 (2019)
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12. R. Kamikawa, E. Yazaki, M. Tahara, T. Sakura, E. Matsuo, K. Nagamune, T. Hashimoto & Y. Inagaki, *Journal of Eukaryotic Microbiology*, vol. 65, 669-678 (2018)
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15. A. Bradley, T. Hashimoto & M. Ono, *Frontiers in Immunology*, vol. 9, 1444 (2018)
16. G. Tanifuji, S. Takabayashi, K. Kume, M. Takagi, T. Nakayama, R. Kamikawa, Y. Inagaki &

T. Hashimoto, *PLOS One*, vol. 13, e0194487 (2018)

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Proceedings (refereed)

1. Y. Nishimura, T. Amagasa, Y. Inagaki, T. Hashimoto & H. Kitagawa, *Proceedings for the 10th International Conference on Complex, Intelligent, and Software Intensive Systems (CISIS-2016)*, 230-237 (2016)

Books

1. 稲垣祐司，中山卓郎．第 17 章　現在も続く細胞内共生細菌のオルガネラ化．共生微生物（化学同人）大野博司編　p190-201 (2016)

Awards

1. Ryo Harada, Best Presentation Award in the 52nd meeting of Japanese Society of Protistology, October 2019
2. Eriko Matsuo, Holz-Conner Travel Award from International Society for Protistologists, July 2017
3. Euki Yazaki, Holz-Conner Travel Award from International Society for Protistologists, September 2015
4. Yuki Nishimura, Holz-Conner Travel Award from International Society for Protistologists, August 2014

6.6 Grants

1. Yuji Inagaki, JSPS Grant-in-Aid for Scientific Research (B), 2019, 3,770,000 yen (17,030,000 yen in total from 2019 to 2023)
2. Yuji Inagaki, JSPS Fund for the Promotion of Joint International Research (Fostering Joint International Research (B)), 2018-2019, 4,940,000 yen (17, 810,000 yen in total from 2018 to 2023)
3. Yuji Inagaki, JSPS Grant-in-Aid for Scientific Research (B), 2016-2019, 17,420,000 yen
4. Yuji Inagaki, JSPS Grant-in-Aid for Scientific Research on Innovative Areas (Research in a Proposed Research Area), 2014-2016, 42,640,000 yen (112,580,000 yen in total from 2011 to 2016)
5. Tetsuo Hashimoto, JSPS Fund for the Promotion of Joint International Research (Fostering Joint International Research (B)), 2019, 4,290,000 yen (18,330,000 yen in total from 2019 to 2023)
6. Tetsuo Hashimoto, JSPS Grant-in-Aid for Scientific Research (B), 2015-2018, 16,900,000 yen

7. Tetsuo Hashimoto, JSPS Grant-in-Aid for Scientific Research (B), 2015-2018, 17,940,000 yen
8. Yoshiyuki Ishitani, JSPS Grant-in-Aid for Scientific Research (C), 2018-2019, 3,900,000 yen (4,420,000 yen in total from 2018 to 2021)
9. Ikuko Yuyama, JSPS Grant-in-Aid for Scientific Research (B), 2019, 5,330,000 yen (15,210,000 yen in total from 2019 to 2022)
10. Ikuko Yuyama, Research Grant from Kurita Water and Environment Foundation, 2018-2019, 950,000 yen
11. Ikuko Yuyama, JSPS Grant-in-Aid for Young Scientists (B), 2016-2018, 2,730,000 yen (4,160,000 yen in total from 2015 to 2018)
12. Takuro Nakayama, JSPS Grant-in-Aid for Young Scientists (B), 2014-2017, 3,900,000 yen
13. Goro Tanifuji, JSPS Grant-in-Aid for Young Scientists (B), 2014-2016, 3,779,000 yen (4,420,000 yen in total from 2014 to 2017; Dr. Tanifuji left the group on March, 2016)
14. Eriko Matsuo, JSPS Grant-in-Aid for JSPS Fellows, 2015-2018, 2,800,000 yen
15. Yuki Nishimura, JSPS Grant-in-Aid for JSPS Fellows, 2014-2016, 2,400,000 yen (3,600,000 yen in total from 2013 to 2016)
16. Euki Yazaki, Grand from the Japanese Science Society, 2015-2016, 820,000 yen
17. Sohta Ishikawa, JSPS Grant-in-Aid for JSPS Fellows, 2014-2015, 900,000 yen (2,700,000 yen in total from 2012 to 2015)

7 Division of Global Environmental Science

7.1 Overview

In the Division of Global Environmental Science, there are four faculties of Prof. Hiroyuki Kusaka, Prof. Hiroshi L. Tanaka, Asst. Prof. Mio Matsueda and Asst. Prof. Quang-Van Doan that joined the CCS 2019. There are two researchers of Dr. Akio Yamagami and Dr. Akifumi Nishi. The division studies global-, synoptic-, meso-, and micro-scale weather and climate, using a global-scale model NICAM, a regional-scale model WRF, and a micro-scale model City-LES. The advanced technology of the supercomputer is used for the high resolution simulations.

Prof. Kusaka's group studies urban climatology and mountain meteorology. They collaborate with the Division of High Performance Computing Systems of the CCS and a private company for weather forecast to develop their own LES model. Prof. Tanaka's group studies general circulation and blocking and Asst. Prof. Matsueda's group studies ensemble forecast for abnormal weather. Studies on urban climate, heat stroke prediction, foehn effect, ensemble forecast, abnormal weather, and climate change contributes to our society as well as the academic one.

The Division of Global Environmental Science extensively collaborates with domestic and international research groups, for instance, Royal Meteorological Institute Belgium, Arizona State University, Vietnam National University, National Center for Atmospheric Research, Alaska University, and Oxford University. The division published 82 journal papers with peer review and obtained 301,604,000 Yen as the grant for 2014-2019.

7.2 Research Results

1) Urban Climatology (Prof. Kusaka)

Kusaka group has been studying urban climatology.

- Urban climate projection and simulation (dynamical downscaling)

- Urban impacts on convective precipitation
- Development of Large Eddy Simulation (LES) model for cities

Urban warming is one of the social problems in Japan. As urban warming has a significant impact on economy and human health, there is a strong demand for urban climate projection at metropolitan scales. Kusaka group has been conducting various urban climate projections using a regional climate model WRF. The urban climate projections considered future urban planning scenarios for Tokyo, Japan (Adachi et al. 2014, Kusaka et al. 2016) and Ho Chi Minh City, Vietnam (Doan and Kusaka 2018). Kusaka group has also evaluated the past urbanization impacts on the regional climate of Sendai, Japan (Vitanova et al. 2019), Sofia, Bulgaria (Vitanova and Kusaka 2018), Ho Chi Minh City, Vietnam (Doan and Kusaka 2016), and Hanoi, Vietnam (Doan et al. 2019). Kusaka et al. (2016) confirmed future urban climate projection with three different urban planning scenarios and showed that the compact city urban scenario can reduce the August mean temperature of surrounding residential areas by 0.4 °C, while the dispersed city scenario can increase the temperature by 0.1 °C. The results indicate that the uncertainties with the urban scenario are significantly less than those in emission scenarios or global climate model projections for the matured city in an advanced country such as Tokyo. On the other hand, Doan and Kusaka (2018) showed that the impact of future urbanization (0.5 °C) is comparable to the difference in temperature increases between GCMs or IPCC scenarios (**Fig. 1**). These results imply that future urban planning scenario should be considered in studies of the urban climate projection of fast growing cities in developing countries.

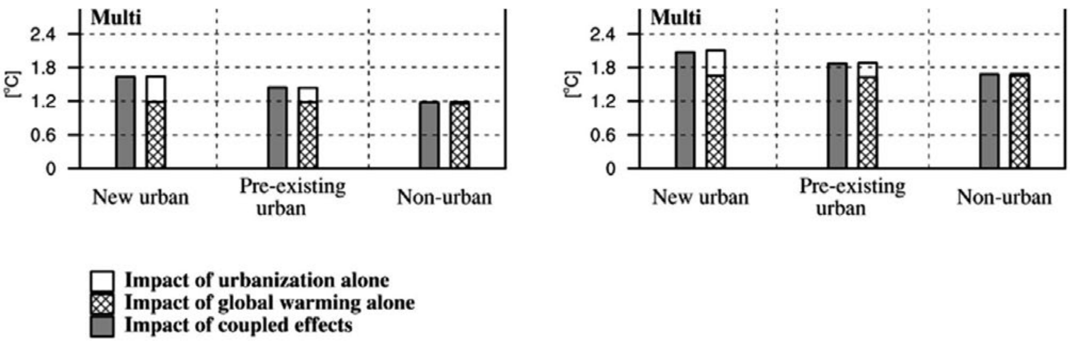

Figure 1 Projected temperature increase in Ho Chi Minh City due to future urbanization, climate change, and coupled effect under the RCP 4.5 and RCP8.5 scenarios (Doan and Kusaka 2018). Left and right panels are RCP4.5 and RCP8.5 secnarios, respectively.

Urbanization has effects on precipitation. Kusaka et al. (2014) conducted that an ensemble, regional climatological simulation approach with sensitivity experiments to reduce uncertainty arising from nonlinearity in the precipitation simulations. The results showed that urbanization causes a robust increase in the amount of precipitation in the Tokyo metropolitan area and a reduction in the inland areas (statistically significant at 99% levels). These precipitation responses are attributed to an increase of surface sensible heat flux in Tokyo, which modifies sea breezes and increases the advection of moisture from the ocean. This mechanism was supported by further research (Kusaka et al. 2019) (**Fig. 2**).

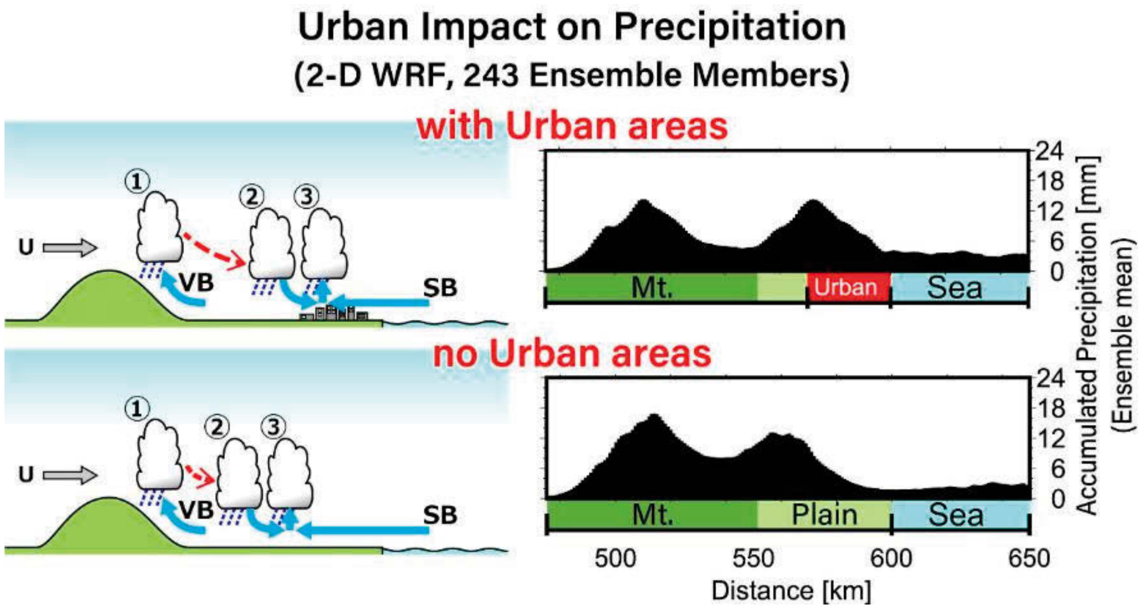

Figure 2 Impact on the convective precipitation revealed by 243 ensemble experiments (Kusaka et al 2019). Left panel is the schematic. Right panel indicates accumulated precipitation from the WRF model with/without urban areas.

Kusaka group has been developing an original Large Eddy Simulation (LES) model for cities. The basic equations consist of momentum equation with Boussinesq approximation, continuity equation, conservation equations for heat, water vapor, cloud, and rain. All physics schemes such as short-wave radiation, long-wave radiation, cloud microphysics, and surface heat budget are included in the LES model. The LES model can resolve the buildings and consider three dimensional radiations in the urban canopy layer and shading effects from buildings and trees. The code is written in Fortran 95 with the MPI and Open MP parallel computing. The code uses three dimensional domain decomposition method for the parallel computing. The LES model has been verified against observations (**Fig. 3**). This study is based on the collaboration between the CCS and Weathernews Inc. that is the largest weather company in Japan.

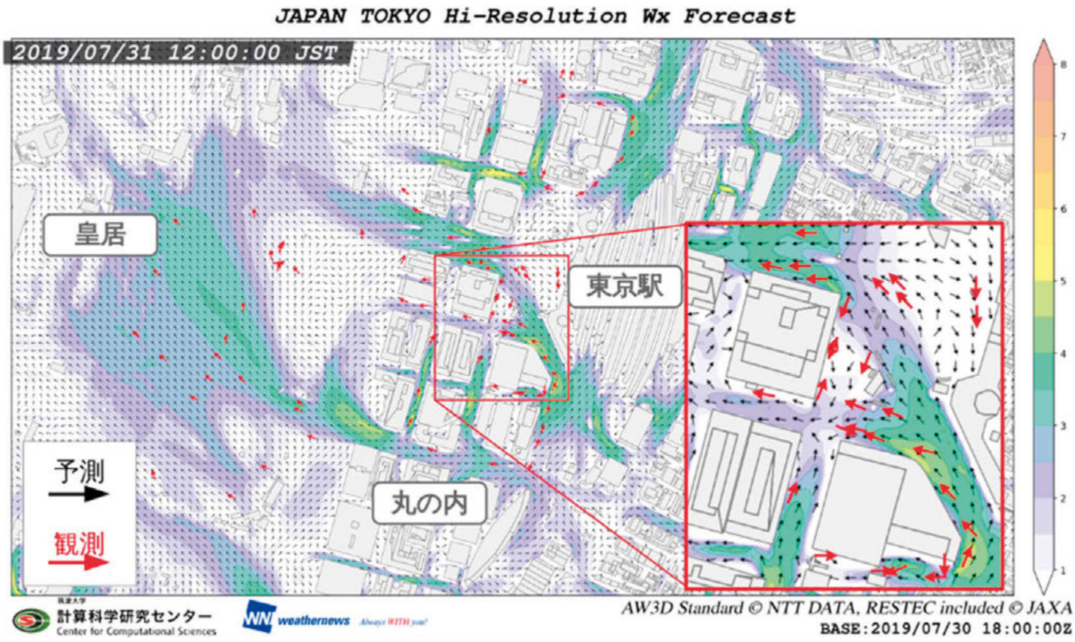

Figure 3 Spatial distribution of the near surface winds around the Tokyo station observations and simulations by the LES model (Created by Weathernews Inc.). Black and red vectors mean simulation and observation, respectively.

Other studies on the urban climatology are as follows; urban impact on fog in Shanghai (Gu et al. 2018), urban impact on heat-wave in New York and Phoenix (Tewari et al. 2019), development of multi-layer urban canopy model (Doan and Kusaka 2019), numerical simulation by the WRF-CFD modeling system (Chatterjee et al. 2019), heat stroke risk prediction in Ho Chi Minh City (Dang et al. 2018) and Tokyo (Suzuki-Parker and Kusaka 2015, 2016, Kayaba et al. 2014), green effects on urban heat island (Okada et al. 2014, 2016), urban heat island simulation of Taipei (Lin et al. 2016), and urban heat island measurement (Okada et al. 2014, Kusaka et al. 2019).

2) Mountain Meteorology (Prof. Kusaka)

Kusaka group has been studying mountain meteorology, especially local winds. The study found that the strongest local wind of Japan is the "Inami-kaze" that blows in Inami town in Toyama Prefecture (Koyanagi and Kusaka 2019). Additionally, they revealed that the Inami-kaze is localized to a surprisingly small region near the Inami town (about 6 km parallel to the mountain ridge and 3 km perpendicular to it), due to the hydraulic jump associated with the mountain wave breaking. Nishi and Kusaka (2019a, 2019c, 2019f) found a new theory of the local winds that there are local winds that are formed by a convex feature in the mountain range (**Fig. 4**).

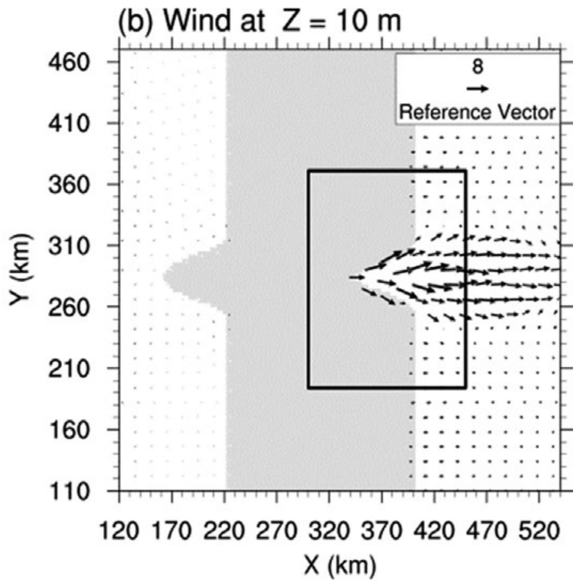

Figure 4 Simulated spatial distribution of the near surface winds around the mountain range with a convex (Nishi and Kusaka 2019).

The study also revealed that the extreme high temperature events were very likely caused by foehn effects (Takane et al. 2017, Nishi and Kusaka 2019b, 2019d, Nishi et al. 2019). Another foehn study found that dynamic foehn with the isentropic drawdown and thermodynamic foehn with latent heating and precipitation occurred in the same event (Takane et al. 2015). Kusaka and Fudeyasu (2017) reviewed and introduced downslope windstorms and foehn winds in Japan.

Other studies on the mountain meteorology are as follows; climatology of extreme high temperature events in Japan (Takane et al. 2014, 2017, Nishi and Kusaka 2019e), climatology of foehn during the Typhoon passage (Suzuki-Parker et al. 2018), climatological study of fog in Japan (Akimoto and Kusaka 2015), wind power prediction with the WRF model and machine learning (Kakimoto et al. 2018), development of the local winds model for wind power prediction (Sato and Kusaka 2018).

3) On the Natural Component of Climate Change (Prof. Tanaka)

We study recent global warming by separating the natural component of climate change from anthropogenic warming. Climate change consists of both natural change and warming (including other possible consequences) by the greenhouse gases. Thus, it is not possible to identify and isolate warming by the greenhouse gases without subtracting natural change from observed temperature change. Without this subtraction process, an accurate prediction of future temperature is not possible. One of the methods to infer natural change is to learn the past climate change. Based on temperature change from about 1800-1850 to 2000, it is shown that there are two prominent natural changes, a near-linear temperature rise of about 1°C from about 1800-1850 to 2000 (0.5°C/100 years, 0.005°C/year or 0.1°C/25 years), which can be interpreted in terms of recovery from the Little Ice Age (LIA). The others are semi-periodic oscillations; one of them is the Pacific Decadal Oscillation (PDO); its amplitude is roughly 0.2°C and its period is about 40 years (the rate of change = 0.02°C/year or 0.5°C/25 years). The combined rise by the two natural components is about 0.6°C (= 0.1°C + 0.5°C) between 1975 and 2000. Since the temperature rise during the same period was about the same (0.6°C), warming by the greenhouse gases is expected to be rather small. In fact, the present halting of temperature rise can be explained by the combined effect of the LIA and PDO, although most computer simulations predict the temperature rise of the range of as large as 0.3°C- 1.2°C by 2020, instead of the observed rise of 0.1°C. Thus, the claim by the IPCC that the temperature increase between 1975 and 2000 is “most likely” due to the effects of the greenhouse gases overestimates greatly warming by the greenhouse gases.

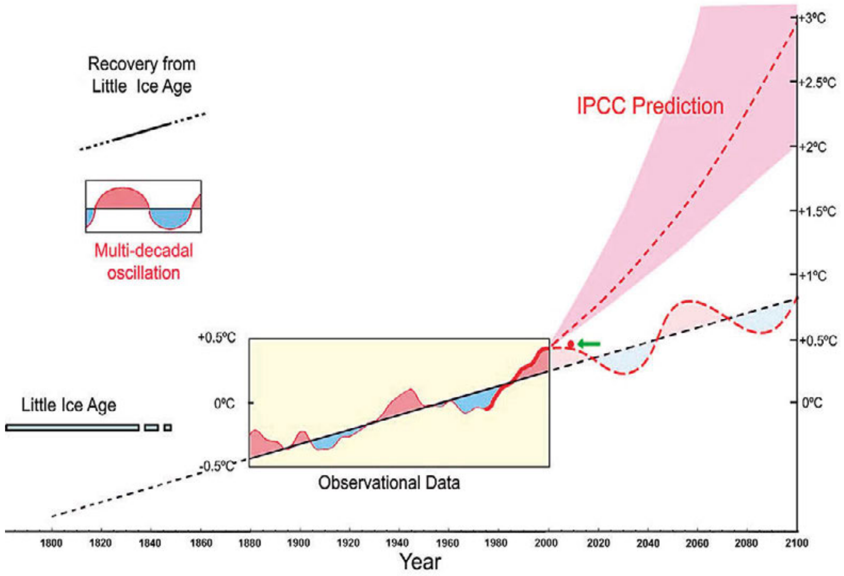

Figure 5 An attempt to construct the global temperature change from 1860 to 2000, which consists of a linear change and the superposed quasi-periodic change. The temperature changes after 2000 is assumed to consist of the two components, LIA and PDO. The changes in the yellow box is the observed ones. The thick red line is the change which was claimed to be effect of the greenhouse gases. The pink change shows various extensions of the thick red line.

4) Volcanic Ash Plume Prediction by PUFF Model for Real-time Aviation Safety (Prof. Tanaka)

In this study, a real-time volcanic ash dispersion model called PUFF is applied to the Sakura-jima volcano erupted on 16 June 2018 to assess the performance of the new system connected with a real-time emission rate estimation. The emission rate of the ash mass from the vent is estimated based on an empirical formula developed for the Sakura-jima volcano using seismic monitoring and ground deformation data. According to the time series of the estimated emission rate, a major eruption occurred at 7:20 JST indicating an emission rate of 1000 t/min and continued for 15 min showing a plume height of 4500 m. It is observed that we need to introduce an adjusting constant to fit the model prediction of the ash fallout with the ground observation. Once the particle mass is calibrated, the distributions of ash fallout are compared with other eruption events to confirm the model performance. According to the PUFF model simulations, an airborne ash concentration of 100 mg/m^3 extends to a wide area around the volcano within one hour after the eruption. The simulation result quantitatively indicates the location of the danger zone for commercial airliners. The PUFF model system combined with the real-time emission rate estimation is useful for aviation safety purposes as well as for ground transportation and human health around active volcanoes.

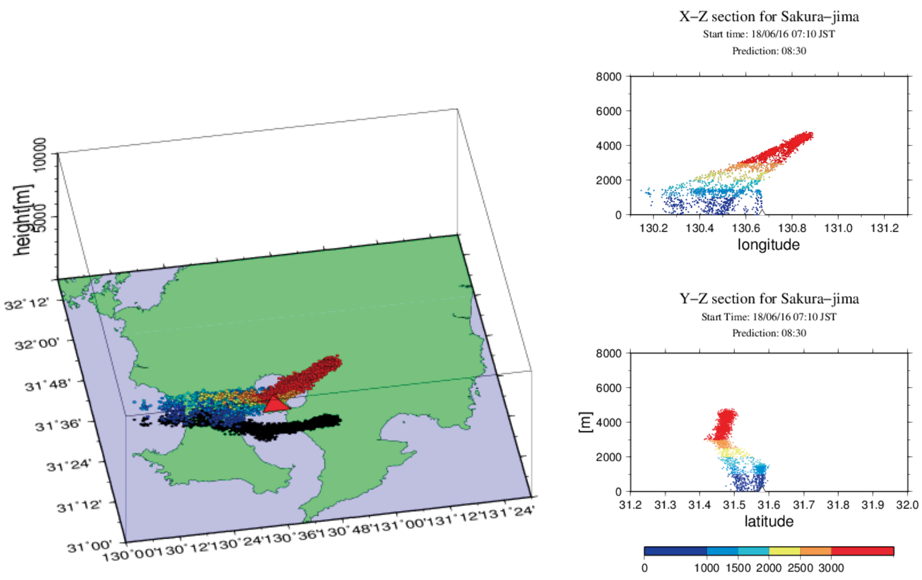

Figure 6 PUFF model simulation of the 3D perspective image of the volcanic ash plume dispersal at 8:30 JST on 16 June 2018. The figure is for 70 min after the beginning of the eruption. The colors of particles indicate a different plume height, and the projection onto the ground is marked by black dots. Line (left). Zonal-height (X-Z) and meridional-height (Y-Z) cross sections of ash plume dispersal (right). and (d) 9:00 JST, respectively. The colors of particles indicate different plume heights.

5) Normal Mode Energetics for Breaking Rossby Waves (Prof. Tanaka)

In this study, Rossby wave breaking and saturation are examined for an idealized situation using a simple barotropic spectral model. In the model, a Rossby wave is amplified by parameterized baroclinic instability. The increase of the wave energy stops at the level where the high and low potential vorticities (PV) indicate overturning. This criterion is represented by the level when meridional PV gradient becomes negative somewhere in the domain. In this study, it is shown theoretically that the criterion may be represented by the point when the wave energy exceeds a quarter of basic state energy in the spectral domain, by assuming a sinusoidal curve for the wave.

Rossby wave saturation above is followed by wave breaking which occurs when the energy level of the background noise becomes comparable to that of harmonic waves of the amplified unstable wave. It is confirmed that the criterion of PV overturning is equivalent to the energy level of wave saturation, and wave breaking is a distinct phenomenon from wave saturation.

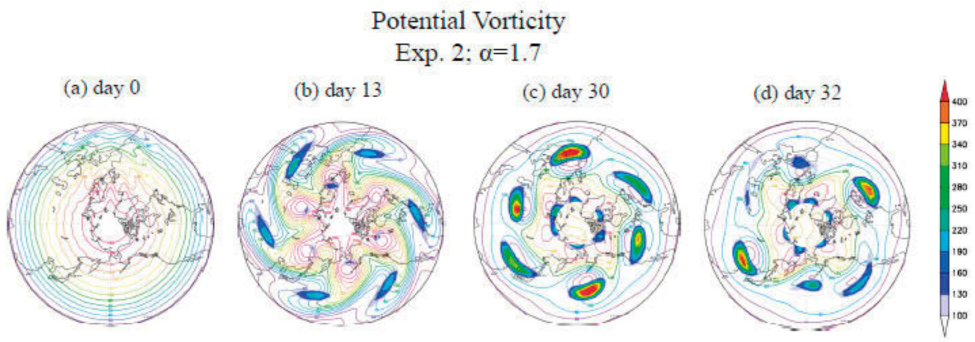

Figure 7 Distribution of potential vorticity (contour) and negative PV gradient (shade) in the Northern Hemisphere for days 0, 13, 30, and 32 for Exp. 2. The waves break down between the days 30 and 32.

6) Analysis of the Structure and Life-cycle of the Arctic Cyclone (Prof. Tanaka)

Arctic cyclones (ACs) are unique cyclones occurring over the Arctic in summer. Overall, ACs have a warm and a cold core at upper and lower levels, respectively, and barotropic vorticity. Furthermore, ACs persist longer compared with mid-latitude cyclones. The baroclinicity over the Arctic frontal zone and the merging of cyclones and subsequent coupling of upper- and lower-level vortices play an important role in the development and maintenance of ACs. Cyclone activity has a large environmental impact over the Arctic. Although the activity is typically weaker in summer than in winter, strong cyclones sometimes occur over the Arctic in summer. Two extraordinary ACs occurred in August 2012 (AC12) and 2016 (AC16), causing sea-ice reduction. In addition, the prediction of AC12 significantly affected the prediction of sea ice. As the Northern Sea Route has become more accessible due to the recent loss of sea ice, planning of ship routes requires accurate prediction of ACs, particularly their positions.

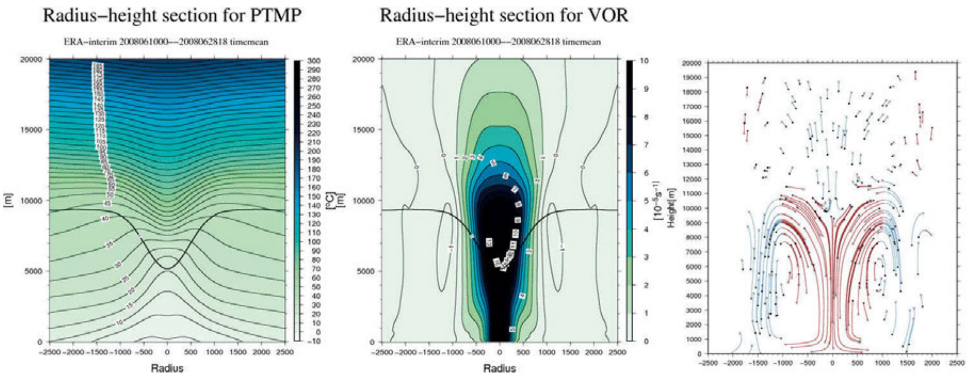

Figure 8 Radius-height section of the structure of the Arctic Cyclone. Left: Potential temperature and the tropopause level. Middle: Relative vorticity and the tropopause level. Right: Vertical motions of rising motion (red) and sinking motion (blue).

7) Predictability of weather regimes (Asst. Prof. Matsueda)

A weather regime is a persistent and/or recurring large-scale atmospheric circulation pattern (**Fig. 9**). Weather regimes are considered as part of the internal variability of the atmosphere and are associated with high-impact weather events (e.g., heatwave, cold spell, heavy rainfall and drought) in surrounding areas. Therefore, the accurate simulation of weather regimes is important in weather and climate predictions. We investigate how well weather and climate models simulate weather regimes.

We assess the forecast skill of Euro-Atlantic and East Asian weather regimes using operational medium-range (i.e. up to 2 weeks) ensemble forecasts from five leading global numerical weather prediction (NWP) centres: CMC (Canada), JMA (Japan), ECMWF (Europe), NCEP (US), and UKMO (UK). The skill depends on initial and/or forecast weather regimes, suggesting flow-dependent predictability of weather regimes. Over the Euro-Atlantic region, for example, the NWP models show the highest skill for forecasts initialised on the negative phase of North Atlantic Oscillation (NAO-) and the NAO- forecasts in recent years. The longer the NAO- events persist, the higher the skill of forecasts initialised on NAO-. The skill dependency on regime duration is less clearly observed for the other regimes. In addition, the models still have difficulties in predicting the onset of blocking (meandering of jet stream).

We also assess the climate models' performance in simulating weather regimes using three state-of-the-art high-resolution climate models (EC-Earth, HadGEM, and MRI-AGCM) under an international collaboration among Universities of Tsukuba, Oxford (UK), Reading (UK), Meteorological Research Institute (Japan) and ISAC-CNR (Italy). We show that the improvement in regime structure due to increased resolution is robust across multiple models with multiple ensemble members. Furthermore, the persistence statistics of the blocking regime did systematically improve. However, the persistence statistics of the other three regimes did not systematically improve.

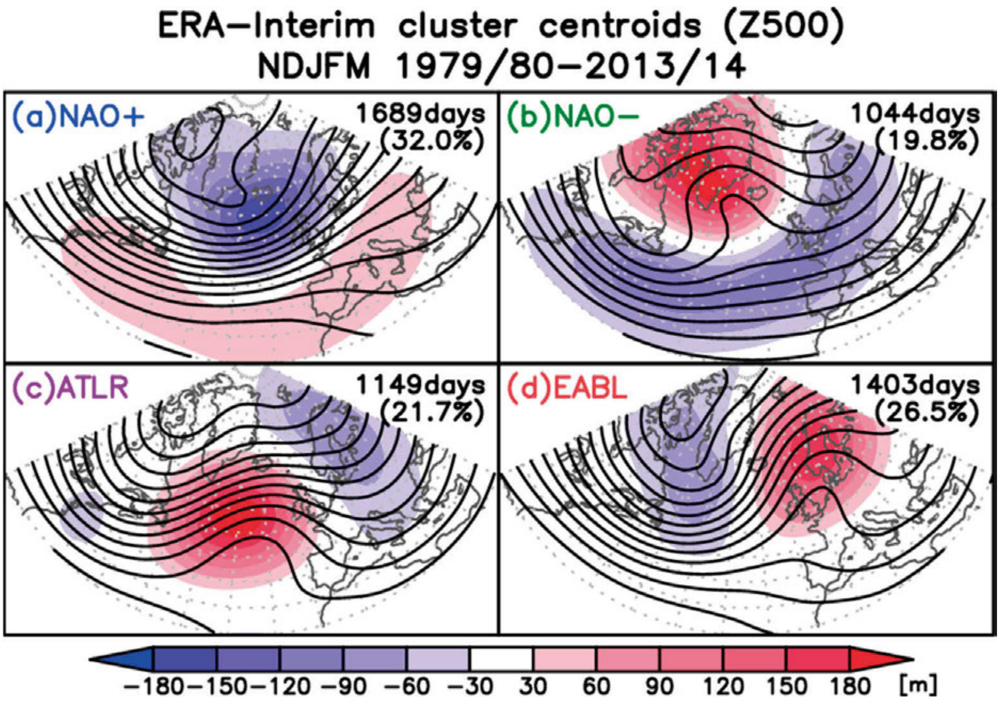

Figure 9 (a–d) Weather regimes over the Euro-Atlantic sector for the extended winters (November–March) of 1979/1980–2013/2014, derived from ERA-Interim: (a) NAO+, (b) NAO−, (c) Atlantic Ridge, and (d) Euro-Atlantic blocking.

8) Extraordinary Arctic cyclones in summer and its predictability (Asst. Prof. Matsueda)

We investigate extraordinary Arctic cyclones (ACs) in summer (June–August) and their predictability using ensemble forecasts. ACs are atmospheric phenomena that severely affect the Arctic environment, like drastic sea ice reduction. As the Northern Sea Route has become more accessible due to the recent loss of sea ice, planning of ship routes requires accurate prediction of ACs, particularly their positions. In addition, the prediction of extraordinary ACs significantly affected the prediction of sea ice. Accurate prediction of ACs is therefore necessary to address associated environmental and socio-economical concerns.

Twenty-six extraordinary ACs were identified for summer seasons during 1986-2016. In particular, we focused on the ACs in August 2012 (AC12) and 2016 (AC16) with the deepest central pressure and the largest size. We revealed that the repeated cyclone merging and associated development of upper-level warm core are important for the persistence and development of the extraordinary ACs. In addition, an accurate prediction of upper-level fields, particularly temperature, was important for the AC prediction.

We also assessed the average forecast skill for the 26 extraordinary ACs in 1986–2016 using medium-range ensemble forecasts (CMC, JMA, ECMWF, NCEP, UKMO) and reforecast (GEFS). Basically, the existence, central pressure, and central position of the extraordinary ACs are predicted well for lead times of ≤3.0 days (**Fig. 10**). The average forecast skills of the 26 extraordinary ACs in 1986–2016 are similar to that of the 10 extraordinary ACs in 2008–2016, indicating that there is no trend of improvements in forecast skills of existence, central pressure and position of the ACs.

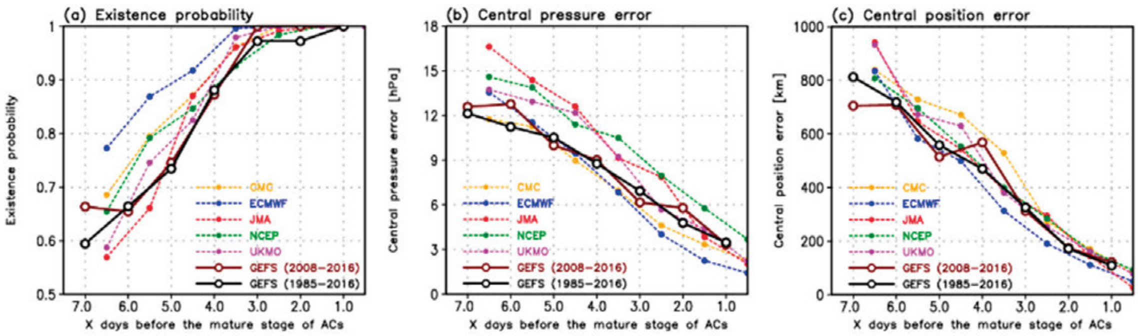

Figure 10 Average (a) existence probability, (b) central pressure error, and (c) central position error during the mature stage of 26 extraordinary ACs in summer during 1986–2016 (black) and 10 extraordinary ACs in summer during 2008–2016 (brown) from the GEFS reforecast, as a function of forecast lead time. Colored broken lines are the probability and errors for the latter 10 extraordinary ACs predicted by CMC, ECMWF, JMA, NCEP, and UKMO.

9) Ensemble simulations with the ECMWF OpenIFS model (Asst. Prof. Matsueda)

We introduced the ECMWF OpenIFS model into the Oakforecst-PACS. The OpenIFS is the easy-to-use version of the ECMWF operational IFS (Integrated Forecasting System). We then established an ensemble prediction system with the OpenIFS model and operational initial conditions in order to quickly respond to severe weather events, including heavy rainfall, tropical and Arctic cyclones and heatwave.

Here is an example. In early July 2018, extremely heavy rainfall events occurred over western Japan. We assess the predictability of these events for the events using three operational medium-range ensemble forecasts (ECMWF, JMA, and NCEP) and ensemble simulations conducted with the OpenIFS model and NCEP ensemble initial conditions. All three operational ensembles predicted extreme rainfall on 5−6 July at lead times of ≤ 6 days, indicating the high predictability of this event. However, the extreme rainfall event of 6−7 July was less predictable. The NCEP forecasts, initialised on 30 June, performed better at predicting this event than the other operational forecasts. The ensemble simulations revealed that the lower predictability of the rainfall in the ECMWF forecasts on 6−7 July can be attributed to the model rather than to the initial conditions. Accurate prediction of the North Pacific Subtropical High is a prerequisite for accurate prediction of such extreme rainfall events.

10) Ensemble forecast products on the S2S Museum (Asst. Prof. Matsueda)

The Subseasonal to Seasonal Prediction (S2S) Project is a proposed World Weather Research Program (WWRP)/THORPEX/ WCRP joint research project. The main goal of the S2S project is to improve forecast skill and understanding on the subseasonal to seasonal timescale, and promote its uptake by operational centres and exploitation by the applications community. In 2015, the S2S data portals started to provide the S2S ensemble forecast datasets from 10 numerical weather prediction (NWP) centres, with a 3-week delay only for research and education purposes. The S2S Museum website (http://gpvjma.ccs.hpcc.jp/S2S/, **Fig. 10**) was established in 2015 and is maintained by Mio Matsueda for non-commercial use, as well as the TIGGE Museum (http://gpvjma.ccs.hpcc.jp/TIGGE/) which is based on operational medium-range ensemble forecasts and is routinely updated every day. The S2S Museum is regularly updated every day, with a 21-day delay and displays a variety of forecast products based on the S2S dataset, including forecasts of

- the Arctic/Antarctic Oscillation (AO/AAO) and North Atlantic Oscillation (NAO) indices;
- teleconnection (PNA, WP, & EU) pattern indices;
- the Sudden Stratospheric Warming (SSW);
- the Madden–Julian Oscillation (MJO);
- sea surface temperature; and
- sea-ice cover.

7.3 Collaboration

Domestic:

1. Study on future urban extreme weather projection with Prof. Masaru Inazu (University of Hokkaido) and Prof. Tetsuya Takemi (University of Kyoto) under the Environment Research and Technology Development Fund of the Environmental Restoration and Conservation Agency of Japan.
2. Study on wind power prediction with Prof. Kazuhiko Ogimoto (the University of Tokyo),

Prof. Hisashi Kato (Nihon University) under the NEDO project.

3. Study on urban air pollution with Dr. Nobuteru Tsunematsu (Tokyo Metropolitan Research Institute for Environmental Protection) under the grants in aid for scientific research.
4. Study on heat stress prediction in Saitama prefecture with Dr. Masayuki Hara (Center for Environmental Science in Saitama) under the regional adaptation consortium project.
5. Study on heat stress projection in Japan with Dr. Yasuaki Hijioka (National Institute for Environmental Study) under the SI-CAT project.
6. Study on urban agriculture with Dr. Atsushi Maruyama (The National Agriculture and Food Research Organization) under the grants in aid for scientific research.
7. Study on fog and clouds with Dr. Mizuo Kajino (Meteorological Research Institute) under the grants in aid for scientific research.
8. Study on future urban expansion in Southeast Asian countries with Dr. Ronald Estoque (National Institute for Environmental Study) under the grants in aid for scientific research.
9. Study on foehn alert system with Dr. Hiroshi Nakagawa (The National Agriculture and Food Research Organization) under the SIP project.

International:

1) Prof. Kusaka

1. Study on urban climate with Dr. Fei Chen (National Center for Atmospheric Research, USA).
2. Study on local winds with Dr. Jason Kneivel (National Center for Atmospheric Research, USA).
3. Study on urban climate with Prof. David Sailor (Arizona State University, USA)
4. Study on heat-wave in Vietnam with Prof. Phan Van Tan (VNU University of Science, Vietnam).
5. Study on foehn in Vietnam with Prof. Ngo-duc Thanh (University of Science and Technology of Hanoi, Vietnam).
6. Study on urban climate with Dr. Rqfiq Hamdi (Royal Meteorological Institute of Belgium, Belgium).

2) Asst. Prof. Matsueda

7. Mio Matsueda has been collaborating with Prof. Tim Palmer and Dr. Antje Weisheimer (University of Oxford, UK), Dr. Susanna Corti (ISAC-CNR, Italy), Dr. Christian Grams's group (Karlsruhe Institute of Technology, Germany) on the predictability of weather regimes and has been collaborating with Prof. Aneesh Subramanian (University of

Colorado Boulder, US) on the predictability of tropical cyclone.

Private Company:

1. Study on LES modeling with Weathernews Inc.
2. Study on wind power prediction with Japan Weather Association.
3. Study on wind simulations with Takenaka Corporation.
4. Study on heat stress projection in Saitama city with Pacific Consultants Co., Ltd.
5. Study on precipitation simulation with Mitsui Consultants Co., Ltd.

7.4 Future Plan

The Division of Global Environmental Science will continue to study various scale meteorology and climatology. Kusaka group is continuing to develop/improve the City-LES model and release it in the near future. They are improving the WRF model to consider the impact of rice field on the regional climate. Additionally, they will investigate the urbanization impact on extreme high temperature and heavy precipitation over the cities in Southeast Asian counties. Mountain meteorology will continue to be studied. Matsueda group will investigate why forecast busts (occasional poor forecasts) occurred on medium-range timescale (up to 2 weeks) using operational ensemble forecast datasets and ensemble simulations with the OpenIFS and the other operational models and operational initial conditions. They will evaluate the forecast skill of operational NWPs and will try to find predictability sources on S2S timescales (up to 2 months).

The division is planning to expand international collaboration to other countries, for instance, China and Austria.

7.5 Publications

Journal Papers (refereed)

1) Prof. Kusaka

1. Okada, M., Kusaka, M. Takaki, S. Abe, Y. Takane, Y. Fuji and T. Nagai, Distribution of air temperature in Tajimi city in summer. Tenki, vol. 61(1), 23-29 (2014)
2. Takane, Y., H. Kusaka, and H. Kondo, Climatological study on mesoscale extreme high temperature events in the inland of the Tokyo Metropolitan Area, Japan, during the past 22 years. International Journal of Climatology, vol. 34, 3926-3938 (2014)
3. Kayaba, M., T. Ihara, H. Kusaka, S. Iizuka, K. Miyamoto, and Y. Honda, Association

between sleep and residential environments in the summertime in Japan. Sleep Medicine, vol. 15, 556-564 (2014)

4. Kusaka, H., K. Nawata, A. Suzuki-Parker, Y. Takane, and N. Furuhashi, Mechanism of precipitation increase with urbanization in Tokyo as revealed by ensemble climate simulations. J. Appl. Meteor. Clim., vol. 53, 824-839 (2014)
5. Okada, M., M. Okada, and H. Kusaka, A Polyethylene Chamber for Use in Physical Modelling of the Heat Exchange on Surfaces Exposed to a Radiation Regime. Boundary-Layer Meteorology, vol. 153(2), 305-325 (2014)
6. Adachi, S. A., F. Kimura, H. Kusaka, M. Duda, T. Yamagata, S, Seya, K. Nakamichi, T. Aoyagi, Moderation of summertime heat-island phenomena via modification of the urban form in the Tokyo metropolitan area. J. Appl. Meteor. Clim., vol. 53, 1886-1900 (2014)
7. Kuno, Y., H. Kusaka, Climatological study of the heavy precipitation around the Nobi plain in summer. Tenki, vol. 61(8), 661-667 (2014)
8. Akimoto, Y., H. Kusaka, A climatological study of fog in Japan based on event data. Atmos. Res., vol. 151, 200-211 (2015)
9. Suzuki-Parker, A., H. Kusaka, Future projection of thermal environment in Japan using WBGT. Japanese Journal of Biometeorology, vol. 52(1), 59-72 (2015)
10. Suzuki-Parker, A., H. Kusaka, Y. Yamagata, Assessment of the impact of metropolitan-scale urban planning scenarios on the moist thermal environment under Global Warming: A study of the Tokyo metropolitan area using regional climate modeling. Advances in Meteorology. Advances in Meteorology, Article ID 693754, 11 pages. (2015)
11. Takane, Y., H. Kusaka, and H. Kondo, Investigation of a recent extreme high-temperature event in the Tokyo metropolitan area using numerical simulations: the potential role of a 'hybrid' foehn wind. Quarterly Journal of the Royal Meteorological Society, 141(690), vol. 1857-1869 (2015)
12. Suzuki-Parker, A., H. Kusaka, Future projections of labor hours based on WBGT for Tokyo and Osaka, Japan, using multi-period ensemble dynamical downscale simulations. Int. J. Biometol. vol. 60(2), 307–310 (2016)
13. Lin, C., C. Su, H. Kusaka, Y. Akimoto, Y. Sheng, J. Huang, and H. Hsu, Impact of an improved WRF urban canopy model on diurnal air temperature simulation over northern Taiwan. Atmospheric Chemistry and Physics, vol. 16, 1809–1822 (2016)
14. Okada, M., M. Okada, and H. Kusaka, Dependence of Atmospheric Cooling by Vegetation on Canopy Surface Area During Radiative Cooling at Night: Physical Model Evaluation Using a Polyethylene Chamber. Journal of Agricultural Meteorology, vol. 72(1), 1-9 (2016)
15. Kusaka, H., A. Suzuki-Parker, T. Aoyagi, S. A. Adachi, Y. Yamagata, Assessment of RCM

and urban scenarios uncertainties in the climate projections for August in the 2050s in Tokyo. Climatic Change, vol. 137 (3), 427-438 (2016)

16. Doan, Q. V., H. Kusaka and Q.B. Ho, Impact of future urbanization on temperature and thermal comfort index in a developing tropical city: Ho Chi Minh City. Urban Climate, vol. 17, 20-31 (2016)
17. Doan, Q. V., and H. Kusaka, Numerical study on regional climate change due to the rapid urbanization of greater Ho Chi Minh City's metropolitan area over the past 20 years. International Journal of Climatology, vol. 36(10), 3633–3650 (2016)
18. Ito A., N. Nakayoshi, T. Yamashiro, K. Ogawa, Y. Takane, H. Kusaka, Examination of the domestic highest temperature outbreak factor in Shimanto-city based on a statistical analysis and the local microatmosphere observation. Japan Science and Technology Information Aggregator Electronic, vol. 72(4), 73-78 (2017)
19. Takane, Y., H. Kusaka, H. Kondo, M. Okada, M. Takaki, S. Abe, S. Tanaka, K. Miyamoto, Y. Fuji and T. Nagai, Factors causing climatologically high temperatures in a hottest city in Japan: a multi-scale analysis of Tajimi. International Journal of Climatology. vol. 37, 1456-1473. (2017)
20. Kusaka, H., H. Fudeyasu, Review of Downslope Windstorms in Japan. Wind & Structures, vol. 24(6), 637-656 (2017)
21. Takane, Y., H. Kondo, H. Kusaka, J. Katagi, O. Nagafuchi, K. Nakazawa, N. Kaneyasu, and Y. Miyakami, Foehnlike wind with a traditional foehn effect plus dry-diabatic heating from the ground surface contributing to high temperatures at the end of a leeward area. Journal of Applied Meteorology and Climatology, vol. 56(7), 2067–2079. (2017)
22. Tomiyama, H., T. Kiyoshi, C. Satoru, K. Shinji, F. Yuji, F. Akiko, S. Kei, F. Akihiro, K. Yoshinori, S. Seiji, M. Yu, H. Masamitsu, O. Hiroyuki, I. Reiko, K. Hiroyuki, T. Akinori, Obesarvation for Temporal Open Burning Frequency and Estimation for Daily Emissions caused by Open Burning of Rice Residue. Journal of Japan Society for Atmospheric Environment Taiki Kankyo Gakkaishi, vol. 52(4), 105-117. (2017)
23. Suzuki-Parker, A., H. Kusaka, Y. Watarai, Characteristics of third typhoon category “high-temperature typhoons” - Comparisons with rain and wind typhoons -. Bulletin of geo-environmental science, vol. 20, 185-191. (2018)
24. Dang, T. N., V. Q. Doan, H. Kusaka, T. S. Xerxes, Y. Honda, Green Space and Deaths Attributable to the Urban Heat Island Effect in Ho Chi Minh City. A Publication of the American Public Health Association, vol. 108(52), S139-S143. (2018)
25. Vitanova, L. L., H. Kusaka, Study on the urban heat island in Sofia City: Numerical simulations with potential natural vegetation and present land use data. Sustainable Cities

and Society, vol. 40, 110-125. (2018)

26. Doan, Q.V., H. Kusaka, Projections of Urban Climate in the 2050s in a Fast-Growing City in Southeast Asia: the Greater Ho Chi Minh City Metropolitan Area, Vietnam. International Journal of Climatology, vol. 38(11), 4155-4171. (2018)
27. Suzuki-Parker, A., H. Kusaka, I. Takayabu, K Dairaku, N. N. Ishizaki, S. Ham, Contributions of GCM/RCM uncertainty in ensemble dynamical downscaling for precipitation in East Asian summer monsoon. SOLA, vol. 14(0), 97-104. (2018)
28. Kakimoto, M., Y. Endoh, H. Shin, R. Ikeda, H. Kusaka, Probabilistic Solar Irradiance Forecasting by Conditioning Joint Probability Method and its Application to Electric Power Trading. IEEE Transactions on Sustainable Energy, vol. 10(2), 983-993. (2018)
29. Suzuki-Parker, A., Y. Miura, H. Kusaka, M. Kureha, Assessing the sustainability of ski fields in southern Japan under global warming. Advances in Meteorology, Article ID 8529748. 10 pages. (2018)
30. Sato, T., H. Kusaka, Reproducibility of Wind Velocity Deficit in Wake Region Using Meteorological RANS model and Wind Turbine Model without Blade Rotation Effect (Comparson with Large-Eddy Simulation Model). Journal of Japan Wind Journal Association, vol. 43(4), 131-142. (2018)
31. Kusaka, H., A. Nishi, M. Mizunari, H. Yokoyama, Urban Impacts on Spatiotemporal Pattern of Short-Duration Convective Precipitation in a Coastal City Adjacent to a Mountain range. Quart. J. Roy. Meteor. Soc., vol. 145, 2237-2254. (2019)
32. Nishi, A., H. Kusaka, Effect of mountain convexity on the locally strong "Karakkaze" wind. J. Meteor. Soc. Japan, vol. 97(4), 787-803. (2019a)
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34. Doan, Q. V., H. Kusaka, T. V. Du, D. D. Nguyen, T. Cong, Numerical approach for studying offshore wind power potential along the southern coast of Vietnam. Lecture Notes in Civil Engineering, Springer, 18, 245-249. (2019)
35. Doan, Q. V., H. Kusaka, M. Matsueda, R. Ikeda, Application of mesoscale ensemble forecast method for prediction of wind speed ramps. Wind Energy, 22, 499-508. (2019)
36. Chatterjee, S., A. Khan, A. Dinda, S. Mithun, R. Khatun, H. Akbari, H. Kusaka, C. Mitra, S. S. Bhatti, V. Q. Doan, Y. Wang, Simulating micro-scale thermal interactions in different building environments for mitigating urban heat islands. Science of the Total Environment, 663, 610-631. (2019)
37. Nishi, A., H. Kusaka, Effect of Foehn Wind on Record-Breaking High Temperature Event

(41.1 degrees C) at Kumagaya on 23 July 2018. SOLA, 15, 17-21. (2019b)

38. Nishi, A., H. Kusaka, Comparison of Spatial Pattern and Mechanism between Convexity and Gap Winds. SOLA, 15, 12-16. (2019c)
39. Vitanova, L. L., H. Kusaka, V. Q. Doan, A. Nishi, Numerical Study of the Urban Heat Island in Sendai City with Potential Natural Vegetation and the 1850s and 2000s Land-Use Data. Journal of the Meteorological Society of Japan, 97(1), 227-252. (2019)
40. Doan, Q. V., H. Kusaka, Development of a multilayer urban canopy model combined with a ray tracing algorithm. SOLA, 15, 37-40. Article ID 2019-008. (2019)
41. Tewari, M., J. Yang, H. Kusaka, F. Salamanca, C. Watson and L. Treinish, Interaction of urban heat islands and heat waves under current and future climate conditions and their mitigation using green and cool roofs in New York City and Phoenix, Arizona. Environmental Research Letters, 14, Article ID 034002. (2019)
42. Doan, Q. V., H. Kusaka, T. M. Nguyen, Roles of past, present, and future urbanization on urban heat island effects in Hanoi, Vietnam: Numerical experiments with a regional climate model. Sustainable Cities and Society, Article ID 101479. (2019)
43. Nishi, A., H. Kusaka, Contributions of Foehn and Urban Heat Island to the Extreme High-Temperature Event in Niigata City during the Night of 23–24 August 2018. SOLA, vol. 15, 132-136. (2019d)
44. Doan, Q. V., V. N. Dinh, H. Kusaka, T. Cong, A. Khan, D. V. Toan, N. D. Duc, Usability and Challenges of Offshore Wind Energy in Vietnam Revealed by the Regional Climate Model Simulation. SOLA, vol. 15, 113-118. (2019)
45. Nishi, A., H. Kusaka, A Climatological Study of the Local “Karakkaze” Wind, with a Focus on Temperature Change. SOLA, vol. 15, 149-153. (2019e)
46. Kusaka, H., K. Igari, R. Kokubo, T. Sato, V. Q. Doan, Impacts of Land Use and Human Activity on Spatial-Pattern Characteristics of Temperature and Heat Index in Central Area of City. E-Journal GEO, vol. 14(1),180-196. (2019)
47. Koyanagi, T., H. Kusaka, A climatological study of the strongest local winds of Japan “Inami-kaze”. International Journal of Climatology, vol. 40, 1007-1021. (2019)
48. Nishi, A., H. Kusaka, The “Karakkaze” Local Wind as a Convexity Wind: A Case Study using Dual-Sonde Observations and Numerical Simulations. SOLA, vol. 15, 160-165. (2019f)
49. Nishi, A., H. Kusaka, L. L. Vitanova, and Y. Imai, Contributions of foehn and urban heat island to the extreme high-temperature event in Niigata city during the night of 23-24 August 2018. SOLA, in press (2019)

2) Prof. Tanaka

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51. Matsunobu, T. and H.L. Tanaka 2019: Time series analysis of normal mode energetics for Rossby wave breaking and saturation using a simple barotropic model. (Atmos. Sci. Let. accepted).
52. Akasofu, S. I., and H. L. Tanaka 2018: On the natural component of climate change. TGS, Vol. 14, pp. 1-7, Dec., 2018.
53. Yamagami, A., M. Matsueda, and H. L. Tanaka, 2018: Predictability of the 2012 great Arctic Cyclone on medium-range timescales. Polar Science, 15, 13-23, doi:10.1016/j.polar.2018.01.002.
54. Yamagami, A., M. Matsueda, and H. L. Tanaka, 2018: Medium-range forecast skill for extraordinary Arctic Cyclones in summer of 2008-2016. Geophys. Res. Lett., 45, doi:10.1029/2018GL077278.
55. Yamagami, A., M. Matsueda, and H. L. Tanaka 2017: Extreme Arctic cyclone in August 2016. Atmospheric Science Letters, DOI: 10.1002/asl.757.
56. Tanaka, H.L., M. Iguchi, and S. Nakada 2016: Numerical Simulations of Volcanic Ash Plume Dispersal from Kelud Volcano in Indonesia on February 13, 2014. J. Disaster Research. 11, 31-42.
57. Yamagami, A. and H.L. Tanaka, 2016: Characteristics of the JRA-55 and ERA-Interim Datasets by Using the Three-Dimensional Normal Mode Energetics. SOLA, 12, 27-31.
58. Aizawa, T. and H.L. Tanaka, 2016: Axisymmetric Structure of the Long Lasting Summer Arctic cyclones. Polar Science (accepted)
59. Zagar, N., J. Boyd, A. Kasahara, E. Kallen, H.L. Tanaka, and J. Yano 2016: Normal modes of atmospheric variability in observation, numerical weather prediction and climate models. (accepted in BAMS)
60. Tanaka, H.L. and M. Tamura, 2016: Relationship between the Arctic Oscillation and Surface Air Temperature in Multi-Decadal Time-Scale. (Polar Science accepted)
61. Hayasaka, H., H.L. Tanaka, and P. Bieniek 2016: Sever fire under high pressure condition in Alaska. (accepted)
62. Kino, K.Y. Shimo, and H.L. Tanaka, 2016, Diagnostic Analysis of the Decadal Variability of the Arctic Oscillation Using the AOI Equation. Tenki, 63, 6, 19-28, (in Japanese).

3) Asst. Prof. Matsueda

63. A. Subramanian et al., Front. Mar. Sci., doi:10.3389/fmars.2019.00427 (2019)
64. K. Strommen et al., Geophys. Res. Lett., vol. 46, 7810-7818, doi:10.1029/2019GL082843 (2019)
65. T. Matsunobu, & M. Matsueda, SOLA, vol. 15A, 19-24. doi:10.2151/sola.15A-004 (2019)
66. A. Yamagami et al., Polar science, vol. 20, 107-116. doi:10.1016/j.polar.2019.02.003 (2019)
67. V.Q. Doan et al., Wind Energy, vol. 22, 499-508. doi:10.1002/we.2302 (2019)
68. B. Vanniere et al., Clim. Dyn., vol. 52, 6817-6846. doi:10.1007/s00382-018-4547-y (2019)
69. N. Nakanowatari et al., The Cryosphere, vol. 12, 2005-2020 (2018)
70. A. Yamagami et al., Geophys. Res. Lett., vol. 45, 4429-4437. doi:10.1029/2018GL077278 (2018)
71. M. Matsueda & T. N. Palmer, Quart. J. Roy. Meteor. Soc., vol. 144, 1012-1027. doi:10.1002/qj.3265 (2018)
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74. A. Yamagami et al., Atmos. Sci. Lett., vol. 18, 307-314. doi:10.1002/asl.757 (2017)
75. M. Matsueda & H. Endo, Geophys. Res. Lett., vol. 44, 5158-5166. doi:10.1002/2017GL073336 (2017)
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77. R. Schiemann et al., J. Climate, vol. 30, 337-358. doi:10.1175/JCLI-D-16-0100.1 (2017)
78. M. Matsueda & M. Kyouda, SOLA, vol. 12, 121-126. doi:10.2151/sola.2016-027 (2016)
79. M. Matsueda et al., J. Climate, vol. 29, 3831-3840. doi:10.1175/JCLI-D-15-0087.1 (2016)
80. T. Jung & M. Matsueda, Quart. J. Roy. Meteor. Soc., vol. 142, 574-582. doi:10.1002/qj.2437 (2016)
81. R. Swinbank et al., Bull. Amer. Meteor. Soc., vol. 97, 49-67. doi:10.1175/BAMS-D-13-00191.1 (2016)
82. M. Matsueda & T. Nakazawal, Meteorol. Appl., vol. 22, 213-222. doi:10.1002/met.1444 (2015)

Proceedings (refereed)

1) Prof. Tanaka

1. Akasofu, S. I., and H. L. Tanaka 2018: On the natural component of climate change. Abstract, Fifth International Symposium on Arctic Research, January 15-18, 2018, Hitotsubashi Hall, Tokyo, Japan, S1-O01.

2. Kurihana, T. and H. L. Tanaka 2018: Analysis of cloud formation process for arctic cyclone in the non-hydrostatic icosahedral grid model. Abstract, Fifth International Symposium on Arctic Research, January 15-18, 2018, Hitotsubashi Hall, Tokyo, Japan, G01-O06.
3. Yamagami, A., M. Matsueda, and H. L. Tanaka 2018: Medium-range forecast skill for Arctic cyclone. Abstract, Fifth International Symposium on Arctic Research, January 15-18, 2018, Hitotsubashi Hall, Tokyo, Japan, S02-O10.
4. Tanaka, H. L., and K. Ito 2018: Multi-decadal variability in planetary albedo. Abstract, Fifth International Symposium on Arctic Research, January 15-18, 2018, Hitotsubashi Hall, Tokyo, Japan, S1-O04.
5. Tanaka, H.L., 2015, Warming Hiatus is Internal Origin, then Global Warming Prediction is Overestimated. J. Heat Transfer Science, Japan, 54, 226, 12-15.

Books

1) Prof. Kusaka

1. The Meteorological Society of Japan, Global Warming-Mechanism and Uncertainty. Asakura Publishing Co., Ltd., 162pp. pp96. (2014)
2. Kodomonokagaku.com., Marvelous story for Science inclined child 365.SEIBUNDO SHINKOSHA, 391pp. pp25, pp270. (2015)
3. Heat Island Institute International., Heat Island Encyclopedia - Understanding of the Mechanism and take measures. Asakura Publishing Co., Ltd., 328pp. pp2, pp38. (2015)
4. Editorial department of Teikoku-Shoin, Study instruction book for Geography teachers. Teikoku-Shoin Co. Ltd., 111pp. (2016)
5. Kusaka. H., 2016: Mienai Taiki wo Miru (Let's see the invisible atmosphere). KUMON PUBLISHING CO., LTD., 159pp. (2016)
6. Kusaka. H., F. Fujibe (Editors), Encyclopedia of Japanese Climate. Maruzen Publishing Co.,Ltd., 516pp., 137-143pp., 144-150pp., 187-194pp., 311-317pp., 467-468pp. , 469-471pp., 477-480pp., 481-483pp. (2018)
7. Yamakawa. H., K. Tokiwa, Y. Watarai (Editors), Encyclopedia of Climate Change. Asakura Publishing Co., Ltd., 472pp., I-9 46-51pp. (2018)

2) Prof. Tanaka

8. Tanaka, H.L., 2017, Atmospheric Science of the Earth, Kyoritsu Pbl. 305 pp.
9. Tanaka, H.L. and Iga, K, 2015, Meteorology for Beginners, Open University of Japan, Textbook, 249 pp.

Awards

1) Prof. Kusaka

1. 2014 Computational Wind Engineering, Poster Award. Takane, Y., Kusaka, H., Kondo, H., Mechanisms of foehn wind and a recent record-breaking high temperature in the Tokyo metropolitan area using the WRF model, 2014 Computational Wind Engineering, (2014)
2. 2018 Students And Young Scientists Award. Sato., T., H., Kusaka, H., Hino, Investigation of Meteorological Aspects for Prediction of Heat Stroke Patients. 57th Annual Meeting of Japanese Society of Biometeorology, (2018)
3. 2018 Atmospheric Environment Society, Best Paper Award. Tomiyama, H., T. Kiyoshi, C. Satoru, K. Shinji, F. Yuji, F. Akiko, S. Kei, F. Akihiro, K. Yoshinori, S. Seiji, M. Yu, H. Masamitsu, O. Hiroyuki, I. Reiko, K. Hiroyuki, T. Akinori, Obesarvation for Temporal Open Burning Frequency and Estimation for Daily Emissions caused by Open Burning of Rice Residue, (2017)
4. 2019 Best Poster Award. Sato, R., T. Sato, H. Kusaka, A. Shimizu, and T. Araki, Development of Prediction Method of Number of Heat Stroke Patients Considering Regionality and Seasonality. 14th Conference on heat island Japan, 2019 (2019)

2) Asst. Prof. Matsueda

5. Certificate of appreciation from the World Meteorological Organization (WMO) (2014, Mio Matsueda)
6. Meteorological Society of Japan Syono Award (2016, Mio Matsueda)
7. University of Tsukuba Young Faculty Award (2017, Mio Matsueda)

7.6 Grants

1) Prof. Kusaka

1. Hiroyuki Kusaka, Development of Regional Climate Projection System (S8), MOE, 2014. 25,950,000 yen
2. Hiroyuki Kusaka, Development of a LES-based New Urban Climate Model (RECCA), MEXT, 2014. 9,200,000 yen
3. Hiroyuki Kusaka, JICA, 2014. 2,000,000 yen
4. Hiroyuki Kusaka, Urban precipitation observations, JSPS Grant-in-Aid for Scientific Research (A), 2014-2017. 900,000 yen
5. Hiroyuki Kusaka, Research and development on adapting technology of power system to

output fluctuation Wind power generation prediction, Control sophistication, NEDO, 2014-2018. 163,421,000 yen

6. Hiroyuki Kusaka, Creation of elucidation and risk information of occurrence realities of Foehn. (SIP), Cabinet Office, 2014-2018. 12,180,000 yen
7. Hiroyuki Kusaka, Social Implementation Program on Climate Change Adaptation Technology (SI-CAT), MEXT, 2015-2019. 19,797,000 yen
8. Hiroyuki Kusaka, Regional Adaptation Consortium Project, MOE, 2017-2019. 10,453,000 yen
9. Hiroyuki Kusaka, Estimation and Mechanism-Clarification of Trade-off in Urban Atmospheric Environment, JSPS Grant-in-Aid for Scientific Research (B), 2017-2019. 1,092,000 yen
10. Hiroyuki Kusaka, Form Factors and Future Prediction of Heat Island Phenomenon in Rapidly Growing Cities in Developing Countries, JSPS Grant-in-Aid for Scientific Research (B), 2018-2019. 1,755,000 yen
11. Hiroyuki Kusaka, RERCA, 2019. 13,000,000 yen
12. Hiroyuki Kusaka, JSPS Grant-in-Aid for Scientific Research (A), 2019. 500,000 yen
13. Hiroyuki Kusaka, JSPS Grant-in-Aid for Scientific Research (B), 2019. 1,300,000 yen

2) Prof. Tanaka

14. Tanaka, H.L., JSPS Grant-in-Aid for Scientific Research (C), 2017-2020, (JP17K05651), 3,400,000 yen.

3) Asst. Prof. Matsueda

15. Mio Matsueda, JSPS Grant-in-Aid for Research Activity start-up, 2014-2015, 2,210,000 yen.
16. Mio Matsueda, JSPS Grant-in-Aid for Young Scientists (B), 2016-2019, 3,510,000 yen.
17. Mio Matsueda, MEXT the Arctic Challenge for Sustainability (ArCS) Project, 2015-2020, 25,000,000 yen.
18. Mio Matsueda, University of Tsukuba – DAAD Partnership Program 2019-2020, 2019-2021, 2,206,000 yen.
19. Mio Matsueda, University of Tsukuba Basic Research Support Program Type B, 2019-2020, 1,000,000 yen.
20. Akio Yamagami, JSPS Grant-in-Aid for Research Activity start-up, 2019-2020, 2,730,000 yen.

8 Division of High Performance Computing System

8.1 Overview

In the Research Division on High Performance Computing System focuses on the entire research on HPC systems including the processor architecture, system architecture, system software, algorithm, application tuning, numerical library and programming language. Through the long history of development of a number of parallel processing systems for HPC, we spread the coverage of our research from the bottom to the top of HPC systems.

Another important mission of our division is to play the central role on procurement, implementation, operation and management of all supercomputer resources at the CCS. As the specialist team for HPC systems, members of our division contribute to these activities which are important issues for codesigning of system and application development in the CCS, supporting from system side. For the codesigning, several members are tightly collaborating with researchers in application fields of the CCS. Especially for these days, one of important topics is how to enhance the performance of applications with accelerators including Many-core processor, GPU and FPGA.

8.2 Research Results

1) OpenCL-enabled GPU-FPGA DMA

Graphics processing units (GPUs) have been widely used in high-performance computing (HPC) systems as accelerators because they can offer good peak performance and high memory bandwidth. However, the GPU does not work well on applications that employ complicated algorithms using partially poor parallelism or frequent inter-node communication. To address this problem, we combine field-programmable gate arrays (FPGAs) with GPUs and make FPGAs not only cover GPU non-suited computation but also perform high-speed communication. This system concept is called Accelerator in Switch (AiS) and we believe that it offers better strong scaling.

One issue to address in realizing this concept is making all devices, particularly GPUs and FPGAs, work together and control their operations. In this research, we've focused on approaches to GPU–FPGA data movement for this issue and proposed a method for high performance direct memory access (DMA) between the two devices. The DMA feature is implemented in an FPGA using a PCIe intellectual property (IP) core and can be controlled using OpenCL code. This research outcome is shown below.

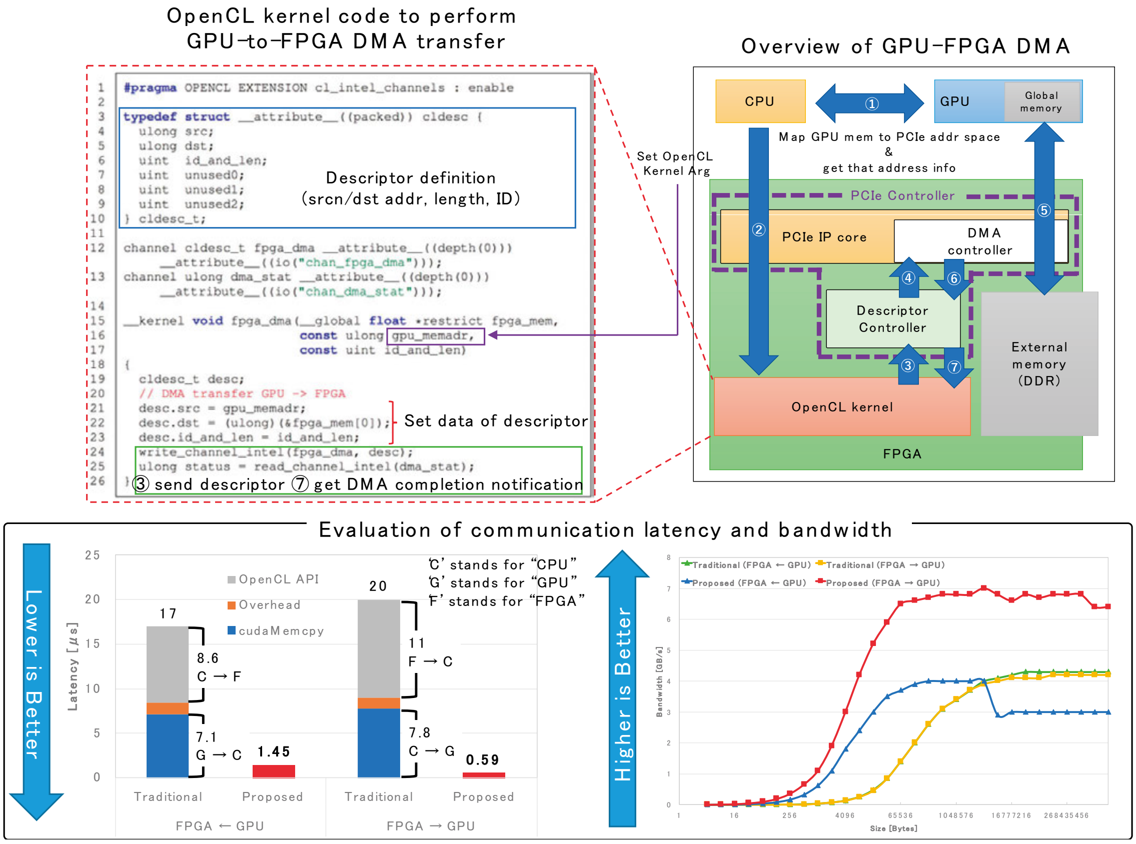

Fig 1. Overview and evaluation results of OpenCL-enabled GPU-FPGA DMA

With this method, application developers can control GPU-FPGA DMA without requiring deep FPGA knowledge and significant engineering effort. From the FPGA to the GPU, our proposed method delivered a transfer rate of up to 7.0 GB/s, 87.5% of the theoretical peak performance. However, from the GPU to the FPGA, there is the degradation in GPU-to-FPGA communication performance and we have discussed this reason with NVIDIA engineers. According to them, this is because of the L2 cache overflow of the GPU and we are currently keeping on this analysis in detail. In summary, we confirmed that in both directions, our proposed method outperformed the traditional one when transferring less than 4 MiB of data, which means that cooperative computation based on short massages is suitable for our proposed method. In case more than 8 MiB data are transferred, the FPGA-to-GPU data movement using our method can still achieve better performance, and when transferring 2 GiB, its effective bandwidth was 6.4 GB/s, 1.5x better than that of the traditional one.

2) Programming for GPU-FPGA cooperative computation

To make GPUs and FPGAs work together and yet be manageable, not only development of hardware aspect such as GPU-FPGA DMA feature shown in 1), but also program development that enables GPU-FPGA cooperative computation with the proposed DMA feature are required. In this research, we have proposed a basic model for performing GPU-FPGA cooperative computation and Fig 2 shows what this research outcome looks like.

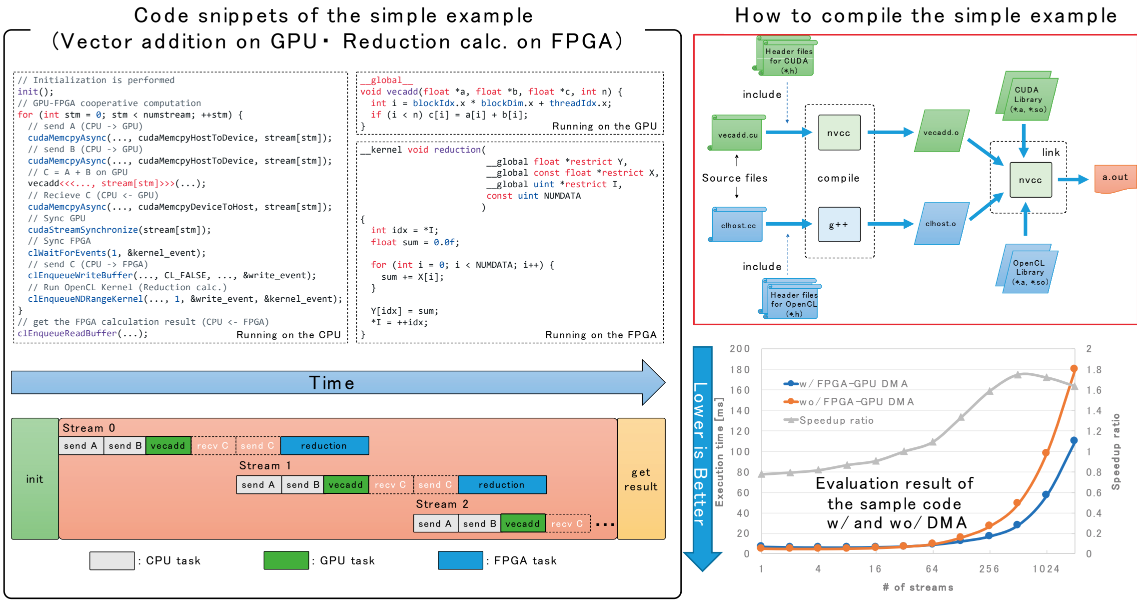

Fig 2. Overview and evaluation results of program development for GPU-FPGA cooperative computation

The simple example was implemented in multilingual programming composed of CUDA and OpenCL, and therefore separate compilation was needed. Fig. 2 shows the flow of the compilation. The CUDA code and OpenCL host code were compiled with nvcc and g++ separately, and the generated object files were linked using nvcc to generate an executable and linkable-format (ELF) file. As an example of GPU-FPGA cooperative computation, we implemented a simple example performing vector addition on a GPU and reduction calculation using the result on an FPGA, and confirmed that the simple example was compiled with the method shown above and both devices worked as intended. We also performed a performance comparison on the simple examples with and without our proposed GPU-FPGA DMA feature and confirmed that our proposed DMA feature is particularly promising in situations where communication overhead is dominant. However, such a multilingual programming (CUDA+OpenCL) puts a heavy burden on application developers and a comprehensive programming framework is required.

Currently, we are developing such a framework with OpenACC because OpenACC code can be compiled for GPU and we are collaborating with Dr. Jeff Vetter's research group organization (Oak Ridge National Laboratory) providing OpenARC compiler (OpenACC compiler for FPGA). In this framework, we assume to use two background compilers, PGI OpenACC compiler for GPU and OpenARC compiler for FPGA. The corresponding OpenACC-directed parts of original code are separated into two parts for GPU and FPGA. Then these parts are compiled by corresponding backend compilers. Finally, two object files are linked to a single executable file by PGI compiler.

To separate OpenACC-directed parts of original code into two parts for GPU and FPGA, we are implementing a meta-compiler with features implemented in XcalableACC Compiler that is derived from Omni Compiler developed by programming language research group in RIKEN R-CCS. Since the meta-compiler is under development, we applied a hand-compilation in our assumed manner from single OpenACC code, then compiled them by PGI compiler and OpenARC. And we confirmed that corresponding parts of the single OpenACC code work on GPU and FPGA respectively. In future work, we will complete the meta-compiler implementation and realize OpenACC-based programming environment that enables GPU-FPGA cooperative computation.

3) Accelerating Space Radiation Transfer Code on FPGA

Accelerated Radiative transfer on Grids using Oct-Tree (ARGOT) is an astrophysics code developed in the Center for Computational Sciences (CCS) at University of Tsukuba. It combines two algorithms to solve radiative transfer problems: the ARGOT algorithm, which computes the radiative transfer from point sources, and the ART algorithm, which computes the radiative transfer from sources spreading out in the target space. Space radiative transfer problem is necessary to analyze an early universe.

In this study, we optimized the ART method for FPGA using OpenCL. The ART method uses ray tracing to compute radiative transfer. Multiple incident rays come from a boundary of the problem domain and move in a straight direction parallel with each other, without any reflection or refraction. Memory access to the mesh data is likely to be random access because memory access pattern depends on a path of a ray and we use multiple "direction" of rays to improve the accuracy. We believe the ART method is suitable for FPGAs because they have a fast on-chip memory called "Block RAM" or "BRAM", which can handle random memory access efficiently.

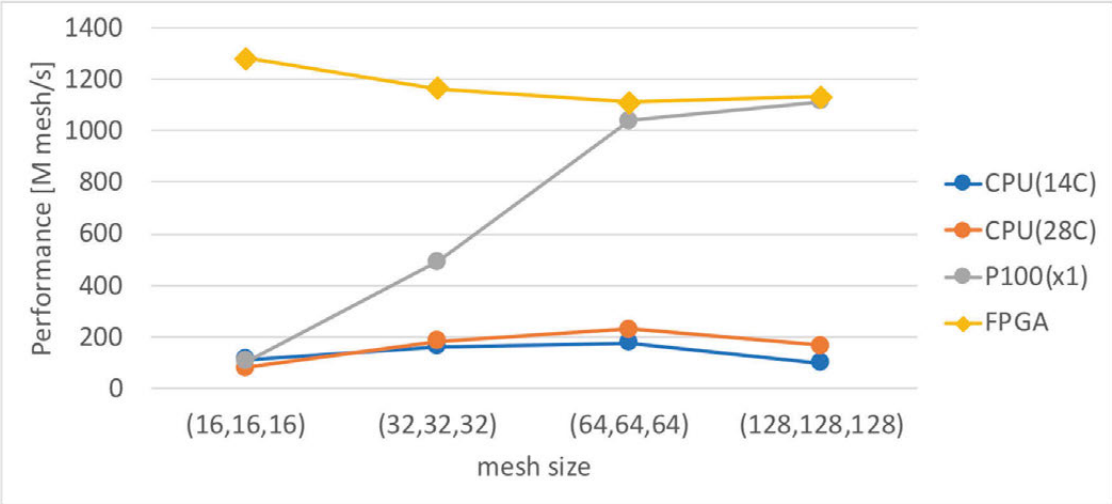

Fig.3 Performance Comparison of the ART method among CPU, GPU and FPGA

We implemented the ART method on an Intel Arria10 FPGA and compared its performance with Intel Xeon CPU and NVIDIA P100 GPU. Using a co-designed method for the optimized programming of a specific application with OpenCL for an FPGA, we achieved a performance that is 6.9 times faster than that of a CPU implementation using OpenMP, and almost the same performance as a GPU implementation using CUDA.

4) GPU–FPGA-accelerated ARGOT code

One reason to need such a GPU–FPGA coupling is to accelerate multiphysics applications. Multiphysics is defined as the coupled processes or systems involving more than one simultaneously occurring physical fields and the studies of and knowledge about these processes and systems. Therefore, multiphysics applications perform simulations with multiple interacting physical properties and there are various computations within a simulation. Because of that, accelerating simulation speed by GPU only is quite difficult and this is why we try to combine GPU and FPGA and make the FPGA cover GPU-non suited computation.

In this research, we focus on radiative transfer simulation code that is based on two types of radiation transfer: the radiation transfer from spot light and the radiation transfer from spatially distributed light as shown in Fig.3 (a). We make GPUs and FPGAs work together, and perform the former radiation transfer on the GPU and the latter radiation transfer on the FPGA. Fig.3 (b) shows what it looks like.

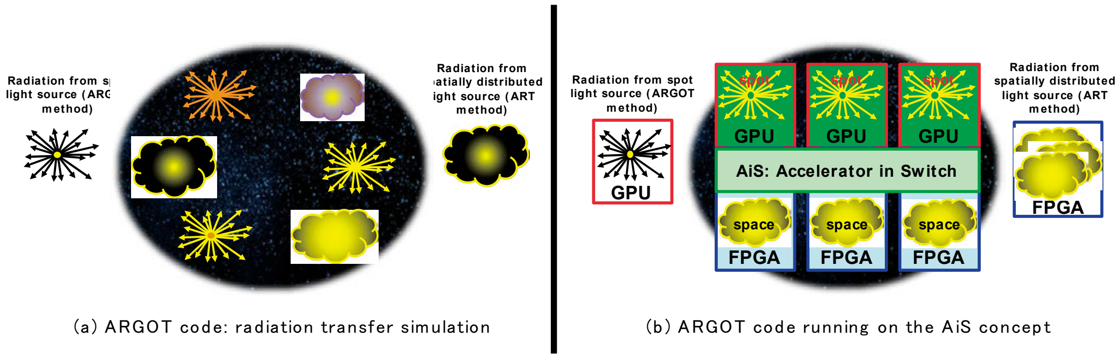

Fig. 4 (a) Overview of the ARGOT code and (b) how to accelerate it by the AiS concept

ARGOT (Accelerated Radiative transfer on Grids using Oct-Tree) is an astrophysics simulation code developed in our organization. As mentioned above, it combines two algorithms to solve radiative transfer problems: the ARGOT algorithm, which computes the radiative transfer from point sources, and the ART algorithm, which computes the radiative transfer from sources spreading out in the target space. The most important point for accelerating the ARGOT code is to efficiently solve the ART algorithm because it accounts for more than 90 % of the ARGOT code. And moreover, this algorithm is unsuitable for SIMD-style processors such as CPUs and GPUs because of its algorithm's characteristics. That is why we decided to offload the ART algorithm to the FPGA and Fig.4 shows the performance comparison between the CPU, GPU, and FPGA implementations.

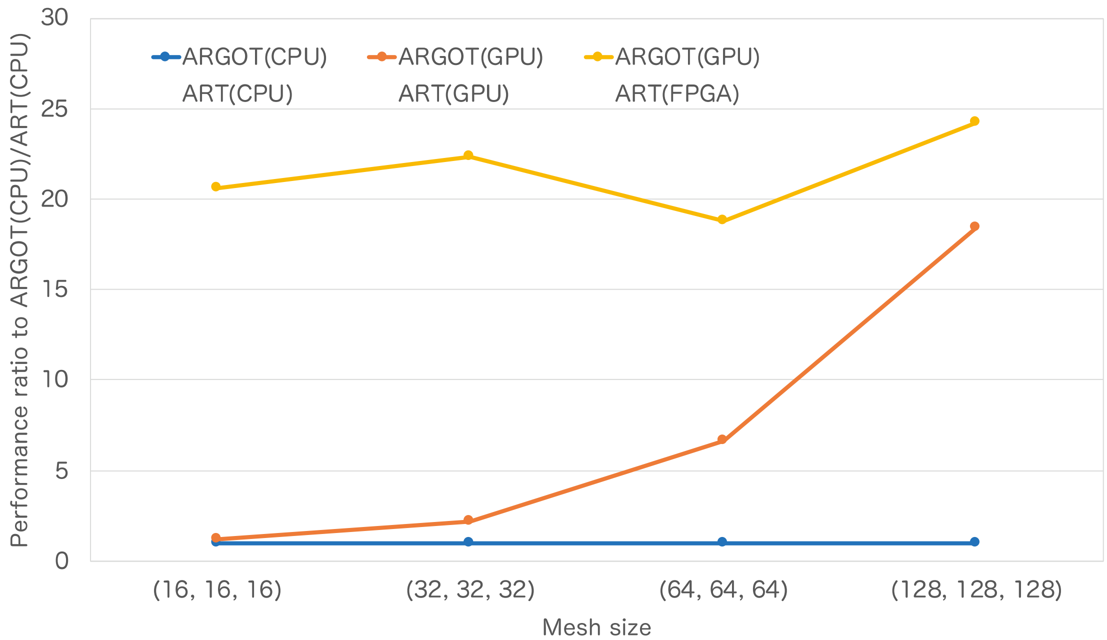

Fig. 5 Performance comparison between FPGA, CPU, and GPU implementations

ARGOT(CPU)/ART(CPU) represents that the both algorithms are the CPU implementation, and the rest graph legends represent each implementation in the same manner. The CPU implementation is written in C and uses OpenMP for the thread parallelization. In this evaluation, we use a single Xeon CPU and the CPU implementation is performed with 14 OpenMP cores (threads). The GPU implementation is based on the CPU implementation but written in CUDA.

Each configuration performance is normalized to ARGOT(CPU)/ART(CPU) performance and this is why ARGOT(CPU)/ART(CPU) performance shown in Fig. 5 is always 1 on any problem size. As shown in Fig. 5, the performance of ARGOT(GPU)/ART(FPGA) and ARGOT(GPU)/ART(GPU) is high for all problem sizes compared to the CPU implementation. Taking a look at ARGOT(GPU)/ART(GPU) and ARGOT(GPU)/ART(FPGA), the latter configuration is 17.4x and 10.2x faster than the former for 16^3 and 32^3 problem sizes, respectively. Their problem sizes are too small for a GPU because of the insufficient parallelism for its 3,584 CUDA cores. And, the latter configuration is still 1.32x faster than the former even when solving 128^3 problem size that is the fastest problem size for the GPU. In summary, as the problem size is smaller, the FPGA becomes the better option to accelerate the ARGOT code, and this tendency is suitable for offering strong scalability. Furthermore, the latest FPGAs (Stratix 10) are equipped with multiple high speed optical communication interfaces, such as 400 Gbps Ethernet unlike the GPU. This strength is also suitable for offering strong scalability.

5) Inter-FPGA Communication

We have proposed a Communication Integrated Reconfigurable CompUting System (CIRCUS) to enable us to utilize high-speed interconnection of FPGAS from OpenCL. We focus on the robust communication functionality of FPGAs. The most recent FPGAs have a communication capacity of up to 100Gbps across 4 channels. The interfaces are directly connected to the FPGA, enabling us to achieve inter-FPGA communication at significantly low latencies.

We considered that direct communication handling is essential for parallel applications, especially for strong-scaled applications. Pipelined communication is the basic concept of the CIRCUS system, and it is also the fundamental data flow structure in an FPGA. The OpenCL compiler makes pipelines from computation loops in the code. To utilize the interconnection feature of the FPGA matched with this pipelining feature, it is the best way to make everything in a pipelined-manner combining them. CIRCUS makes a fused single pipeline combining the computation and the communication, which hides the communication latency by completely overlapping them.

We use Intel SerialLite III intellectual property (IP) as a data link layer protocol. Because SerialLite III is a direct communication protocol, we cannot communicate with the non-neighbor

FPGAs. To solve this problem, we implement a router mechanism in the system.

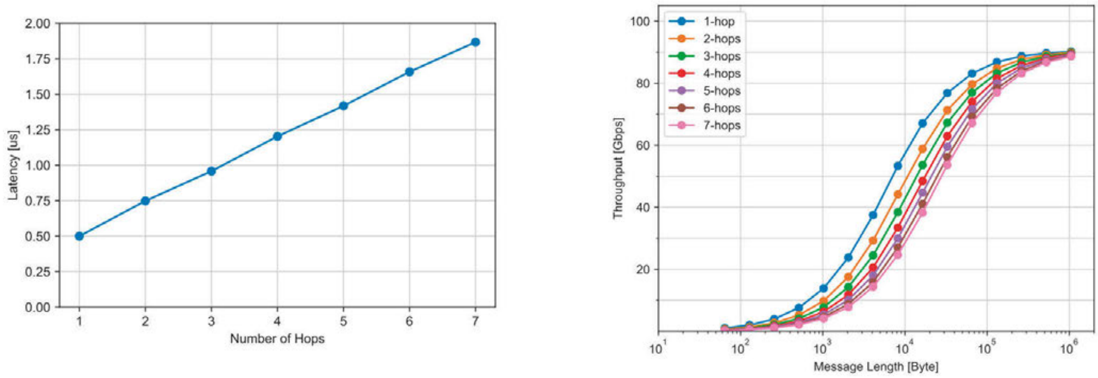

Fig. 6 Performance Evaluation Result of the CIRCUS system using pingpong benchmark

We evaluated the fundamental performance of the CIRCUS system by using the pingpong benchmark. We implemented the benchmark on two FPGAs. They exchange data with each other through the network. Furthermore, we measured the time required for communication on the OpenCL kernel. Therefore, the benchmark results include the communication time as well as the OpenCL overhead in the CIRCUS backend. According to the pingpong benchmark results, the minimum latency was 0.5µs, and the maximum throughput was 90.2Gbps, and the additional latency per hop was approximately 0.23µs.

6)High-Performance Numerical Library

As a research on high-performance numerical library, Prof. Takahashi joined to a project of “An Evolutionary Approach to Creation of a Software Development Environment for Massively-Parallel Computing Systems” (led by Prof. Takizawa, Tohoku University) as a JST-CREST program from 2011 to 2016. In the project, we contributed to the development of high-performance numerical libraries to fully exploit the performance of large-scale heterogeneous computing systems.

We developed numerical libraries to hierarchically abstract HPC system configurations. Our numerical libraries are optimized for multiple platforms, such as GPU, the Intel many integrated core (MIC) architecture, and standard CPU cluster systems, so that application developers can use different implementations with common interfaces, resulting in high performance-portability. The numerical libraries are designed to support as many data structures as possible to cover various use cased while achieving high performance. We also investigate auto-tuning technologies to adapt the optimized implementations of numerical libraries to similar platforms in order to achieve high performance-portability.

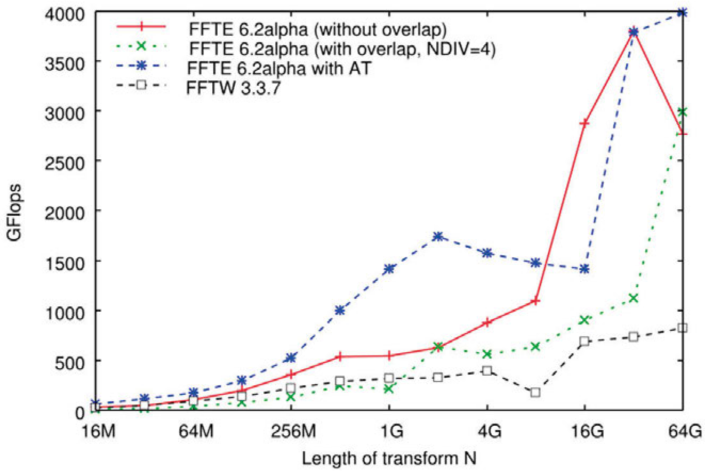

Fig. 7 Performance of parallel one-dimensional FFTs on the Oakforest-PACS (1024 nodes)

7) System Software for Data-Intensive Science

System Software research for Data-Intensive Science has been supported by JST/CREST "System Software for Post Petascale Data-Intensive Science" (PI: Osamu Tatebe) from 2011 to 2017, and JST/CREST "Extreme Big Data (EBD) – Next Generation Big Data Infrastructure Technologies Towards Yottabyte/Year" (PI: Satoshi Matsuoka) from 2013 to 2019, and JSPS Grant-in-Aid for Scientific Research (B) "Research of System Software for Big Data Machine Learning towards Prediction of Extreme Weather" (PI: Osamu Tatebe) from 2017 to 2019. This research includes distributed file system, database, workflow engine, big data framework, and big data applications. For data-intensive science applications, the performance of storage is major concern. We solve this issue by utilizing compute node-local NVMe SSD.

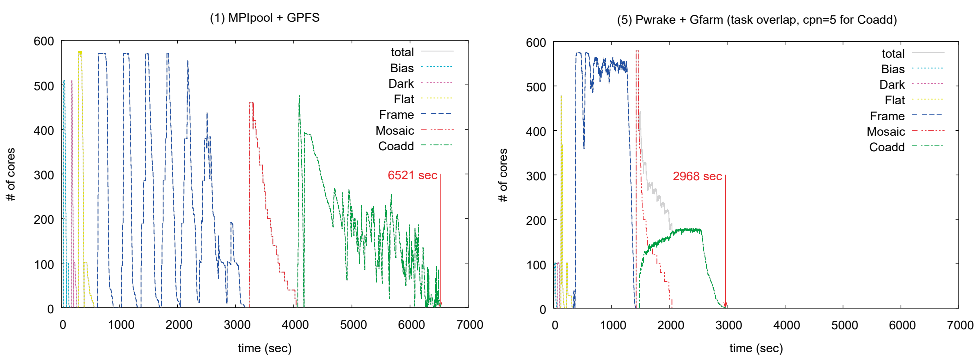

Fig. 8 Execution of Subaru HSC sky survey pipeline. Left figure is the original execution, and right figure is improved execution by Pwrake workflow engine.

There is a proposed standard interface for NVMe SSD, called OpenNVM, which provides sparse address and atomic batch operations for block devices. Using this interface, we designed PPOST object storage based on fixed-size object region. It achieves 747,000 object creations per second, that is 12 times faster than DirectFS, 7 times faster than RocksDB, and 4.3 times faster than NVMKV. The result was published by the Journal of Information Processing in 2016. For the distributed metadata servers, we designed PPMDS metadata server by exploiting distributed transaction based on dynamic software transactional memory. It achieves 270,000 file creations per second using 15 servers, which is 2.8 times faster than GIGA+ with 32 servers. The design paper of PPMDS received the best paper award in 2018. Regarding workflow research, we developed disk cache-aware scheduling that improved the workflow execution performance by 1.9 times in Astronomical Montage workflow, which was published in IEEE Cluster 2014. We also improved Subaru HSC sky survey pipeline workflow by Pwrake workflow engine. By overlapping independent tasks, the execution was improved 2.2 times. The result was published in IEEE Cluster 2018.

8) HPCI Storage

Operation and software development of HPCI storage has been supported by MEXT. HPCI storage is a 100PByte Japanese nation-wide storage shared among HPCI resource providers including 9 national supercomputer centers and RIKEN R-CCS, AIST, and JAMSTEC. It is a distributed storage located in RIKEN R-CCS and the University of Tokyo.

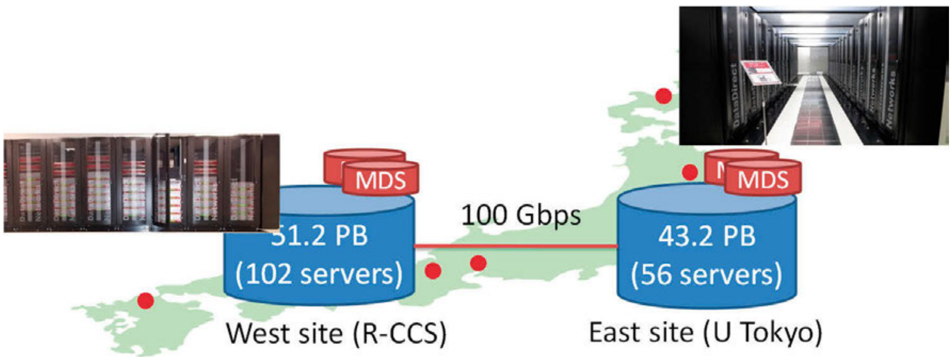

Fig. 9 HPCI Storage

The HPCI storage utilizes Gfarm file system we have been developing as an open-source software. Major features include scaled-out performance and capacity, no single-point-of-failure, and data integrity support for silent data corruption.

9) Development of high accurate Block Krylov subspace methods

As research on the development of numerical computation methods, we studied high accurate Block Krylov subspace methods for linear systems with multiple right-hand sides. The Block Krylov subspace methods may solve these linear systems more efficiently in terms of the computation time and the number of iterations than Krylov subspace methods for linear systems with a single right-hand side. However, when the number of right-hand sides is large, the accuracy of approximate solutions generated by the Block Krylov subspace methods may degrade due to the error which occurs in the computation of matrix-matrix multiplication.

To avoid the accuracy degradation of the approximate solutions, we developed several high accurate Block Krylov subspace methods by reconstructing recursions. The Block GWBiCGSTAB method with residual orthonormalization (Block GWBiCGSTABrQ) is one of high accurate Block Krylov subspace methods we developed. The Block GWBiCGSTABrQ method is based on the group-wise updating technique. By using this technique, the computations which cause accuracy degradation can be avoided.

The performance of the Block GWBiCGSTABrQ method is shown in the following graphs. As a test problem, the linear system derived from lattice QCD calculation (matrix size: 1,572,864) is used. To evaluate the accuracy of the obtained approximate solution, the true relative residual norm is used. If this value is sufficiently small, then the accuracy of the obtained solution is good. By using the Block GWBiCGSTAB method, a more accurate approximate solution can be obtained than the Block BiCGSTABrQ method. Moreover, the elapsed time per L of the Block GWBiCGSTABrQ method is almost the same as that of the Block BiCGSTABrQ method.

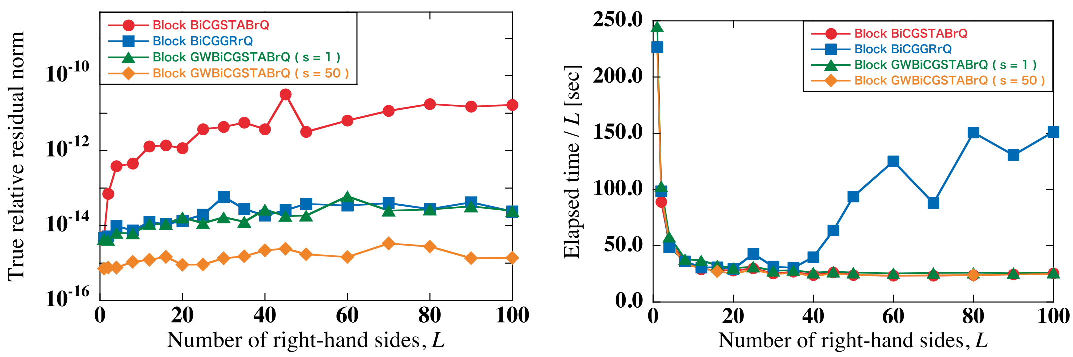

Fig. 10 True relative residual norm as a function of the number L of right-hand sides (Left), the number of iterations as a function of the number L of right-hand sides (Right).

10) Performance improvement of application codes under in-house collaboration

We are collaborating with research divisions in the CCS on scientific application fields. In these days, we especially focus on how to apply accelerators such as many-core processor, GPU and/or FPGA for high performance/power computing compared with general CPU computing. One extremely advanced work is reported in this document as Subsections 3) and 4) in this section to introduce FPGA or GPU+FPGA cooperation on astrophysics code (ART and ARGOT). Here, several other research collaboration results are shown.

10-a) SALMON code porting to many-core architecture and GPU

SALMON (Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience) is an original code developed in the CCS, mainly in Research Division on Quantum Condensed Matter Physics. SALMON is an advanced simulation code to handle first-order computation based on Real Space Real Time Density Function Theory (RSRTDFT) with high scalability. The original code is described in ordinary OpenMP+MPI form, and our division contributed to introducing Intel Xeon Phi (Knights Landing) many-core processor on the Oakforest-PACS under JCAHC. We successfully improved the performance up to approximately 25% of theoretical peak of entire system with 8192 nodes in 2017.

As well known, the performance tuning on Xeon Phi is not simple since it is required to consider various issues such as how to use 512-bit vector instruction, up to four hardware threads to hide the long instruction latency and increase the memory bandwidth utilization, data allocation on MCDRAM and DDR memories, etc. Since the interconnection network of Oakforest-PACS introduces Intel Omni-Path Architecture (OPA), it is critical to increasing the number of communicating threads to utilize the potential bandwidth of network.

As a result of collaborative performance tuning, we achieved a good strong scaling and weak scaling on up to 8192 nodes (8192 Knights Landing processors) on Oakforest-PACS. In the weak scaling, the sustained performance is up to 25% of theoretical peak, which looks very high ratio of this processor. Fig. 11 shows the performance result on 128, 1024 and 8192 nodes of calculation.

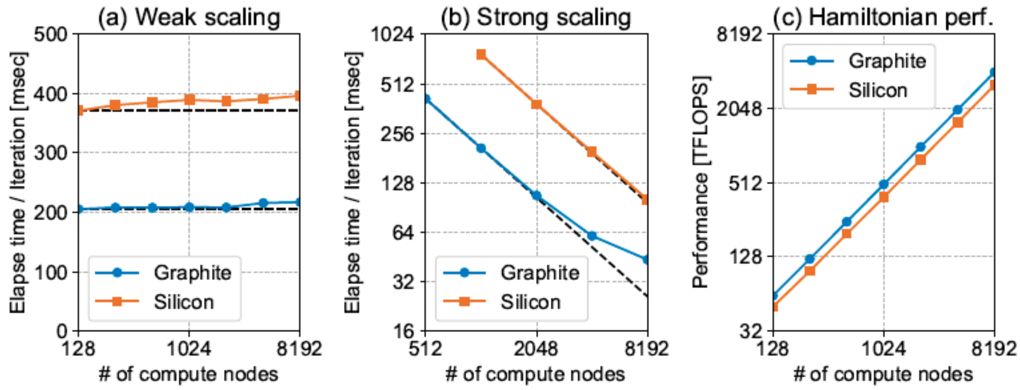

Fig. 11 Strong and weak scaling performance on SALMON code optimized on Oakforest-PACS System (Intel Xeon Phi 7250 processor for each node)

After the optimization on Knights Landing processor, we shifted to the code for GPU clusters such as Cygnus System in the CCS. In recent GPU computing, the programming by traditional CUDA (for NVIDIA) or OpenCL (for AMD) is transitioned to OpenACC, especially for NVIDIA GPUs. Since most of codes today are written by OpenMP+MPI combination, it is slightly easier to introduce OpenACC rather than CUDA for partially rewriting for GPU from original CPU codes. Data movement between CPU and GPU memories is also quite easy on OpenACC directive especially with ver.2.0 feature on data section. We applied the OpenACC modification on the core part of SALMON based on the OpenMP version.

Fig. 12 shows the strong scaling performance comparison between CPU and GPU on Cygnus System. Each node of Cygnus is equipped with 24 cores (12 cores x 2 sockets) of Intel Xeon Gold with 2.6GHz frequency and four NVIDIA Tesla V100 GPUs (PCIe version). In both versions of code, we utilize entire CPU cores or GPUs, and scale the system from 1 node to 32 nodes. When increasing the number of nodes, the problem domain size is reduced to decrease the parallelism in each MPI process, so that the efficiency of GPU version rapidly reduced. We evaluated the MPI communication cost and confirmed that it is negligible in this case of calculation, thus the performance degradation is mainly caused by a lack of parallelism to utilize entire cores of GPUs. It is shown as by solid lines in the figure to represent the parallel efficiency compared with single node case. In most of cases, GPU code performs approximately 7.5x - 4.0x faster than CPU version. Even in the hardest case with 32nodes, it is faster than CPU version with 2.3x of factor.

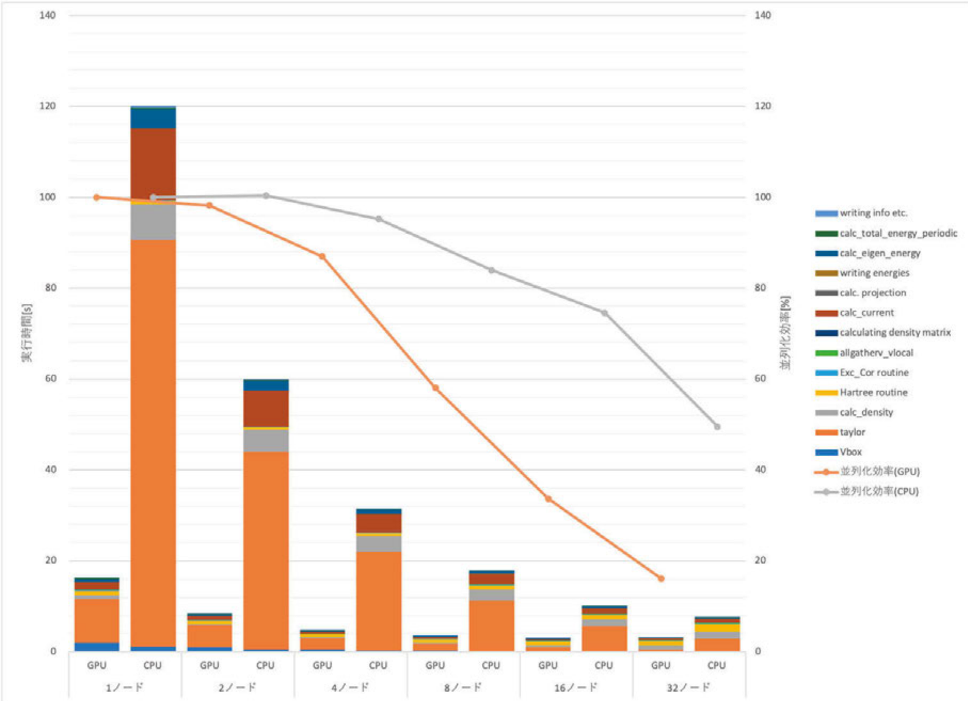

Fig. 12 Strong scaling from single to 32 nodes on Cygnus running SALMON code.

10-b) City-LES code porting to GPU cluster

GPU code implementation is especially important for climate simulation because it basically depends on the memory bandwidth required for 3D stencil computation on each node. Also the code for that part is almost regular without exception of conditional branch, so that the characteristics of computation are very suitable for GPU computing. In Research Division on Global Environmental Science, a code named City-LES has been developed for very detailed high density simulation of Large Edy Simulation (LES) in city size. Our divison and these researchers have been continued long term collaboration, and recently we successfully ported the original OpenMP+MPI code with OpenACC+MPI for GPU computing.

The key issue here is how to reduce the data copy between CPU and GPU memories. Since the SIMD-style parallelization and utilization of high memory bandwidth work quite well on GPU code and we achieve very high performance improvement with approximately 10x of factor from CPU to GPU. However, the last bottleneck of performance is the overhead caused by CPU-GPU data copy. Before making OpenACC code, we worked on CUDA version which requires handful work even on simple loop construction. Thus, we decided to modify all parts regardless what is the maximum parallelism of these parts. What we mean is that we run any part on GPU even if it is not speeding-up the execution time of that part because it may take longer time when we manage the data movement between CPU and GPU. Each GPU on Cygnus System is NVIDIA

Tesla V100 with 32GB of global memory which equips larger memory capacity helps us to place all the data on GPU memory with aggregated 128GB of capacity on each node (CPU memory of each node is 192 GB).

Under this policy, we completed to port entire parts in the iterative calculation of City-LES code to achieve much higher performance than CPU. Figs. 13 and 14 show the performance scaling on Cygnus System with strong and weak scaling cases, respectively. Here the computing time comparison between original CPU version and GPU version is shown. For strong scaling, we scale the system from 4 nodes to 32 nodes. Each node of Cygnus is equipped with 24 cores (12 cores x 2 sockets) with 2.6GHz frequency of Intel Xeon Gold and four NVIDIA Tesla V100 with 32 GB global memory. In either CPU or GPU case, we utilize entire computation resources. Here, the GPU code achieves 10x to 4.7x of performance compared with CPU version. When the number of nodes increases, the parallelism on each node reduces and the efficiency of GPU utilization degrades the performance. For the weak scaling case, 9.4x - 9.1x of higher performance than CPU.

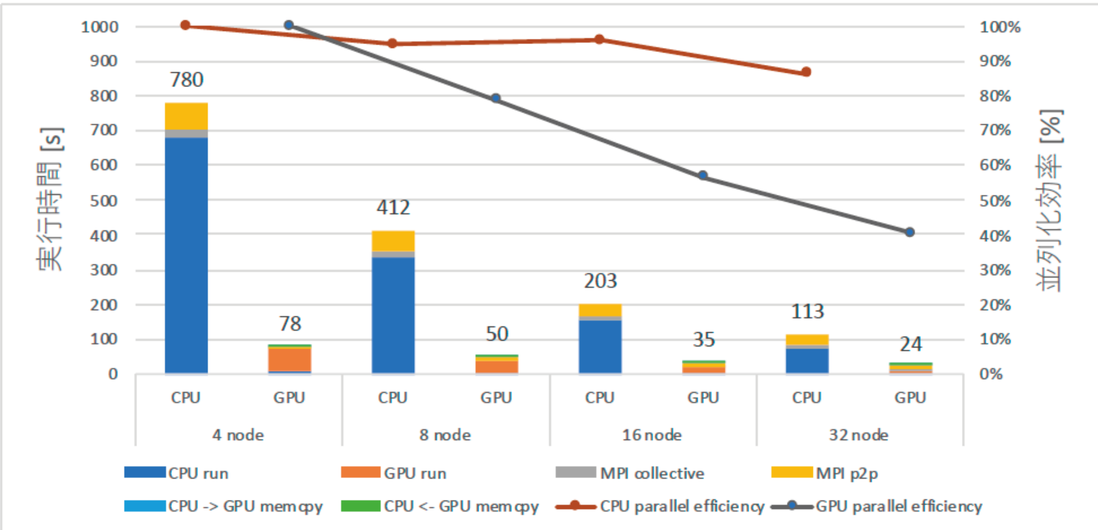

Fig. 13 Performance comparison of City-LES between CPU and GPU versions on 4 to 32 nodes strong scaling (left index shows the execution time and right index shows the parallel efficiency)

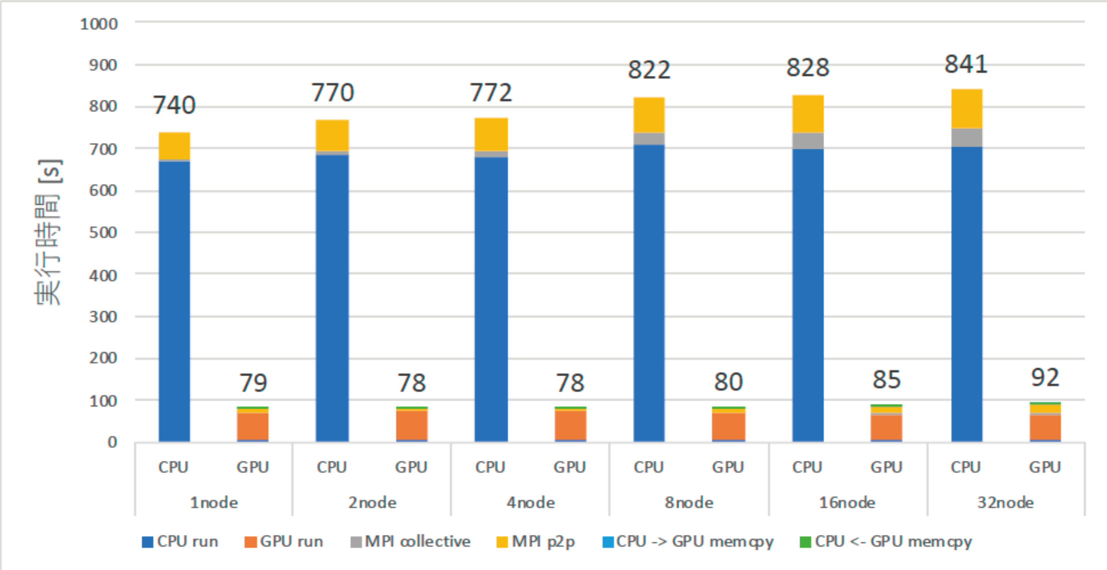

Fig. 14 Performance comparison of City-LES between CPU and GPU from single to 32 nodes in weak scaling

In conclusion, our collaboration with climate research group developed more than 9 times faster code than CPU to utilize GPUs on Cygnus System to lead their research to more productive one.

11) Architecture design on Fugaku supercomputer

Two members of our research division, Taisuke Boku and Daisuke Takahashi, have been involved into the design and performance evaluation on Post-K "Fugaku" supercomputer as a member of its architecture design working group with core members in RIKEN R-CCS which is the headquarter of Fugaku Research and Development Project. We have been evaluating the basic feature of Fugaku CPU which was finalized as Fujitsu A64FX many-core processor based on Arm ver.8 design and a special instruction concept named Scalable Vector Extension (SVE), the interconnection network Tofu-D feature on several target applications.

Our experience on development of large scale supercomputers contributed to the design and performance evaluation of Fugaku, the next generation national flagship supercomputer in Japan. Our knowledge on the architectural characteristic on A64FX processor also leads several in-house codes optimized for Fugaku. An example is SALMON code developed for many-core architecture (KNL) has been ported to A64FX and under evaluation on a testbed system of Fugaku with thousands of nodes already.

8.3 Collaboration

1. Under the MEXT-DoE system software collaboration, we collaborate with Argonne National

Laboratory and Oak Ridge National Laboratory for FPGA utilization for HPC and file I/O system (2016 - now).

2. Under the RIKEN and U. Tsukuba collaboration for Post-K supercomputer development, we are developing the task scheduling aware compiler with accelerators with GPU and FPGA, CPU and interconnection network performance evaluation on Fugaku supercomputer (2016 - now).
3. Under FP3C research collaboration between Japan and France, we collaborated with Maison de la Simulation of CNRS, University of Versailles and RIKEN R-CCS for accelerated PGAS programming (2013-2016).
4. Under SPPEXA phase 2 research collaboration in Japan, Germany and France tri-literal joint work, we collaborated with RWTH Aachen in Germany, Maison de la Simulation under CNRS in France, University of Versailles in France, and RIKEN R-CCS for large scale programming framework on PGAS and task flow languages (2016-2019).
5. JLDG is a joint research with KEK, Nagoya University, Kyoto University, Osaka University, Hiroshima University and RIKEN.

8.4 Future Plan

HPC Research Division has been continuing the research on two view points; our original research for high performance computing technology as a computer science research, and collaboration with application fields of research division in the center mainly focusing on performance tuning and scaling of real applications.

For the computer science research, we will continue the research on our coverage from the architecture and hardware of HPC, middleware for storage and communication, large scale numerical algorithm and library. We especially focus on the accelerated computing by various accelerating devices including GPU and FPGA as much more than today for practical use of these devices in harmony toward next generation accelerated HPC. Our research on Cygnus system for this research is a unique activity in the world, and we will continue it. For the storage system, our research on large scale high performance and distributed storage system is practically applied for Gfarm to support HPCI shared storage in Japan, and we will continue toward higher performance and scalability. Numerical algorithm including FFT and Block Krylov subspace method can be applied for various problems including in-house applications in CCS. We will proceed the research not just on the basic element but also for real applications in and out of CCS.

For the collaboration with application research divisions, it is one of the most important elements on our center's unique formation where system and application fields collaborate toward true codesigning. In addition to the collaboration for traditional general purpose large scale systems, we are proceeding the research on multi-accelerated hybrid system such as Cygnus as the most advanced HPC system. It is hard challenge to implement real applications with this concept, but we will continue it under a strong partnership with application research divisions.

8.5 Publications

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2. Taisuke Boku, et. al. "Chapter 15: GPU-Accelerated Language and Communication Support by FPGA" in "Advanced Software Technologies for Post-Peta Scale Computing: The Japanese Post-Peta CREST Research Project (English Edition)" (edited by Mitsuhisa Sato), 20 pages, 2019.
3. Daisuke Takahashi: Fast Fourier Transform Algorithms for Parallel Computers, Springer (2019).
4. Daisuke Takahashi: Fast Fourier Transform in Large-Scale Systems, Masaaki Geshi (Ed.): The Art of High Performance Computing for Computational Science, Vol. 1, Springer, pp. 137-168 (2019).
5. Hiroyuki Takizawa, Reiji Suda, Daisuke Takahashi, and Ryusuke Egawa: Xevolver: A User-Defined Code Transformation Approach to Streamlining Legacy Code Migration, Mitsuhisa Sato (Ed.): Advanced Software Technologies for Post-Peta Scale Computing, Springer, pp. 163-181 (2019).
6. Osamu Tatebe, Yoshihiro Oyama, Masahiro Tanaka, Hiroki Ohtsuji, Fuyumasa Takatsu, and Xieming Li, Chapter 6, System Software for Data-Intensive Science, Advanced Software Technologies for Post-Peta Scale Computing, Springer, pp.99-120, 2019
7. Taisuke Boku, Osamu Tatebe, Daisuke Takahashi, Kazuhiro Yabana, Yuta Hirokawa, Masayuki Umemura, Toshihiro Hanawa, Kengo Nakajima, Hiroshi Nakamura, Tsuyoshi Ichimura, Kohei Fujita, and Yutaka Ishikawa, Mitsuhisa Sato, Balazs Geroff, Masamichi Takagi, Chapter 16, Oakforst-PACS, Contemporary High Performance Computing: From Petascale toward Exascale, Volume 3, CRC Press, pp.401-422, 2019

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2. 小林 諒平、計算力時代到来...スパコン技術研究コーナ ソート専用コンピュータ最前線 Interface 2017年2月号 緊急特集 本家ARMのIoTワールド入門,、pp.163-167、2017-02
3. 小林 諒平、第6章 Appendix 2 基本演算の高速化が重要！ハードウェア並列ソート・アルゴリズム Interface 2016年12月号 IoT＆スパコン！ラズパイ時代の自分用コンピュータ作り、

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4. 小林 諒平、 第6章
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Awards

1. Best Paper Award, Kohei Hiraga, Osamu Tatebe, Hideyuki Kawashima, "PPMDS: A Distributed Metadata Server based on Nonblocking Transactions", Workshops collocated with the Fifth International Conference on Social Networks Analysis, Management and Security (SNAMS 2018) and the Fifth International Conference on Internet of Things: Systems, Management and Security (IoTSMS 2018), 2018
2. Best Paper Award, Yasuhiro Nakamura, Hideyuki Kawashima, Osamu Tatebe, "Integrating TicToc with Parallel Logging", The 6th International Workshop on Computer Systems and Architectures, 2018
3. Best Technical Talk Award, Hiroki Ohtsuji, Osamu Tatebe, “Breaking the Trade-off between Performance and Reliability of Network Storage System”, PRAGMA29, Depok, Indonesia, Oct. 7, 2015
4. Hiroshi Maeda and Daisuke Takahashi: 16th International Conference on Computational Science and Its Applications (ICCSA 2016), NVIDIA Best Paper Award, July 2016.
5. HPC in ASIA poster award.　Norihisa Fujita, Ryohei Kobayashi, Yoshiki Yamaguchi, Makito Abe, Kohji Yoshikawa, Masayuki Umemura, “Accelerating HPC applications on FPGAs using OpenCL and FPGA Network”, 2019.
6. Asia HPC Leadership Award, Taisuke Boku, Supercomputing Asia 2020, 2020.

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- 2015年度日本応用数理学会論文賞JSIAM Letters部門，J. Asakura, T. Sakurai, H. Tadano, T. Ikegami, K. Kimura, A numerical method for nonlinear eigenvalue problems using contour integrals, JSIAM Letters, Vol. 1, pp. 52—55, 2009.

8.6 Grants

1. Taisuke Boku, JSPS Grant-in-Aid for Scientific Research (B), 2018-2020, 13,300,000 yen
2. Taisuke Boku, "Program for High Performance General Purpose Supercomputer Utilization" by MEXT, with the name of "Research and Development of Next Generation

Computation and Communication Unified Supercomputer", 2017-2021, 95,000,000 yen

3. Taisuke Boku, JST CREST, 2013-2018, 348,988,000 yen
4. Taisuke Boku, SPPEXA, 2016-2019, 35,493,500 yen
5. Daisuke Takahashi, JSPS Grant-in-Aid for Scientific Research (C), 2019-2021, 3,510,000 yen
6. Daisuke Takahashi, JSPS Grant-in-Aid for Scientific Research (C), 2016-2018, 4,030,000 yen
7. Daisuke Takahashi, JSPS Grant-in-Aid for Scientific Research (C), 2012-2015, 4,290,000 yen
8. Osamu Tatebe, JST CREST, 2012-2017, 224,469,700 yen
9. Osamu Tatebe, JST CREST, 2013-2018, 49,894,000 yen
10. Osamu Tatebe, JSPS Grant-in-Aid for Scientific Research (B), 2017-2019, 18,590,000 yen
11. Osamu Tatebe, NEDO, 2018-2020, 20,397,000 yen
12. Osamu Tatebe, Fujitsu Laboratories Ltd., 2018, 3,564,000 yen
13. Osamu Tatebe, Fujitsu Laboratories Ltd., 2019, 3,630,000 yen
14. H. Tadano, JSPS Grant-in-Aid for Young Scientists (B), 2015-2016, 2,600,000 yen
15. Ryohei Kobayashi, JSPS Grant-in-Aid for Early-Career Scientists, 2019-2020, 3,380,000 yen

9 Division of Computational Informatics: Database Group

9.1 Overview

In the past few years, “big data” has become a ubiquitous term. Today, big data is tightly combined with machine learning and AI technologies, and has been giving huge impacts on many aspects of human life and society. To address technical issues and challenges involved in big data, data engineering is one of the key disciplines, and we have studied a wide variety of topics in data engineering. Especially, we have conducted our research from the viewpoints of (1) information integration framework, (2) data mining and knowledge discovery, and (3) XML, open data, and privacy. We have also collaborated with researchers and engineers in other disciplines and fields inside and outside CCS to apply our competence to tackle issues and problems in their domains.

Our research topics in the category of information integration framework include stream processing, stream OLAP, sequence data analysis, and multi-dimensional object search. Data mining and knowledge discovery topics cover outlier detection, microblog/social media analysis, graph analysis, NMF, community detection, and data analysis using GPU and FPGA. The category of XML, open data, and privacy includes XML streams, facet search, RDF, knowledge base, LOD, privacy, and anonymization.

We have also worked on database applications and data science under strong collaboration with researchers in other disciplines and fields. The first topic is joint research on automatic sleep state scoring in sleep medical science with International Institute for Integrative Sleep Medicine (IIIS), University of Tsukuba. CCS launched a new project of Computation Medical Science in 2018. The theme of big sleep data analytics and automatic sleep diagnosis is one of the major research themes in the Computation Medical Science project. Our group is strongly committed to this research topic. The second topic is bioscience data analysis in collaboration with Division of Life

Sciences, CCS, and Graduate School of Life and Environmental Sciences, University of Tsukuba. We also collaborated with Tsukuba city, Fujisawa city and other research universities and industries in research and field trials for smart cities.

9.2 Research Results

1) Information Integration Framework

(1-1) Stream Processing

Data stream processing has become an important research issue with the increase in stream sources, i.e., sensors, micro-blogs, etc. To process the streams, several Stream Processing Engines (SPEs) have been developed which execute continuous queries (CQs) to process continuous data streams.

Smart Query Execution for Event-driven Stream Processing

Event-driven stream processing continuously gets the incoming stream data however generates query results only on the occurrence of specified events. In the basic query execution scheme, even when no event is raised, input stream tuples are continuously processed by query operators, though they do not generate any query result. This results in increased system load and wastage of system resources. For this problem, we proposed a smart event-driven stream processing scheme, which makes use of smart windows to buffer the stream tuples during the absence of an event. When the event is raised, in Figure 9 at timestamp t_3, the buffered tuples are flushed and processed by the downstream operators. If the buffered tuples in the smart window expire due to the window size before the occurrence of an event, they are deleted directly from the smart window, hence resulting in reduced system load and improved system throughput.

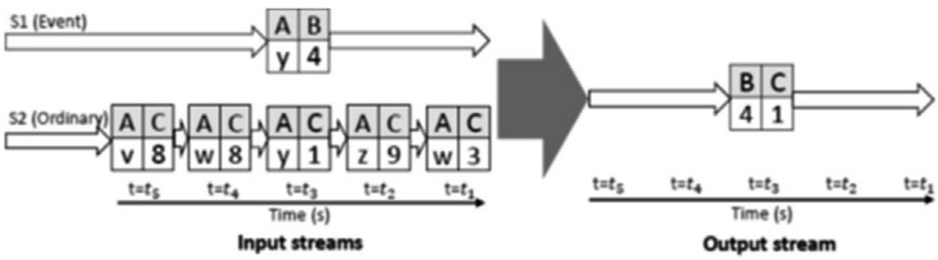

Figure 9 Smart Event Driven Stream Processing

Incremental CQ Processing over Streams and Relations with Isolation Guarantees

Many stream processing systems need to reference non-streaming resources such as database relations to answer real world queries. Since database relation is a shared entity, it may be updated during the CQ execution by other database clients resulting in inconsistent query results. For this problem, we proposed an incremental CQ processing approach with isolation guarantees which makes use of a monitor operator to transform the relational updates into stream tuples. Since database relations tend to be large, an in-memory T*-Tree index is used to increase the stream-relation join efficiency.

Smart Distributed Query Execution over Data Streams

Many organizations require on-line processing of their data for real-time analysis and actionable alerts. It is not possible to process such voluminous and velocious data in real-time using the traditional centralized stream processing engines. Hence distributed stream processing has emerged to facilitate such large-scale real-time processing. In this work we presented a smart distributed event-driven stream processing approach. The proposed smart distributed event-driven stream processing utilizes the concept of smart query execution, discussed above, to distribute the data stream among the distributed worker nodes in the presence of events only; while in the absence of events no data is distributed as it cannot generate query output. This can significantly reduce the network traffic in the absence of events and ultimately results in improved system throughput.

Keyword Search over Relational Streams

Keyword search over relational streams is useful because it allows users to query on streams without knowing the details of the streams and query language. The state-of-the-art approaches exploit Candidate Networks (CNs), which are schema-level descriptions of possible joining networks of tuples, and generate query plans based on CNs. Then, the query plan is evaluated against the relational streams and returns the matched results. The performance of existing approaches seriously degrades when the query contains more keywords and/or the streams have many relations due to the explosive increase in the number of CNs. However, it is observed that edges of all CNs are intensively duplicated from the foreign/primary-key relationships in the schema of the streams, which is in general comparatively small. To cope with the mentioned performance bottleneck, it is possible to consolidate the edges sharing the same primary/foreign-key relationship into one edge when generating a query plan. By taking this idea into account, we proposed a novel query plan called MX-structure to consolidate all common edges among all CNs. In addition, we proposed novel node buffer management so that MX-structure can efficiently track the matching statuses of all intermediate results for each CN. Therefore, MX-structure allows all common edges among CNs to share processing as much as possible. The proposed processing framework is shown in Figure 10. The experimental results on both real and synthetic datasets prove that the proposed algorithm performs much better than the state-of-the-art approaches.

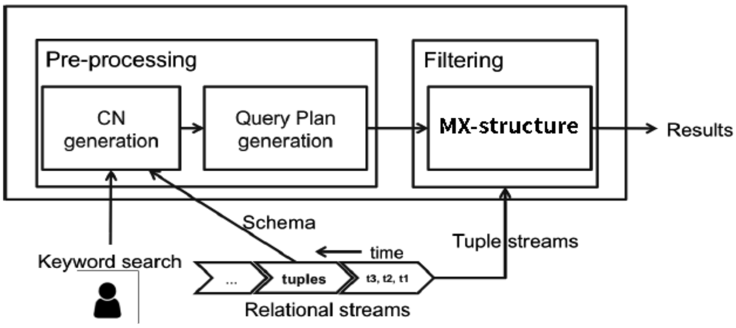

Figure 10 Keyword Search over Relational Streams

(1-2) Stream OLAP

Many organizations require detailed and real-time analysis of their business data for effective decision making. Online Analytical Processing (OLAP) is one of the commonly used methods for the analysis of static data and is equally effective for data streams.

Architecture for Stream OLAP Exploiting SPE and OLAP Engine

With the increase in streaming data sources, many applications require their real-time analysis. However, tailor-made systems for such applications is not always desirable due to high developing costs and long developing periods. Hence, this work proposed a novel architecture for OLAP over streams exploiting off-the-shelf SPE combined with OLAP engine, as shown in Figure 11. It allows users to perform OLAP analysis over streams for the latest time period, called Interval of Interest (IoI). To cover arbitrary aggregation levels using limited system's memory, we proposed to partially deploy CQL queries for those with higher reference frequencies, whereas the results are dynamically calculated using existing aggregation results with the help of OLAP engine. For optimal CQL query deployment, we proposed a cost-based optimization method that maximizes the performance.

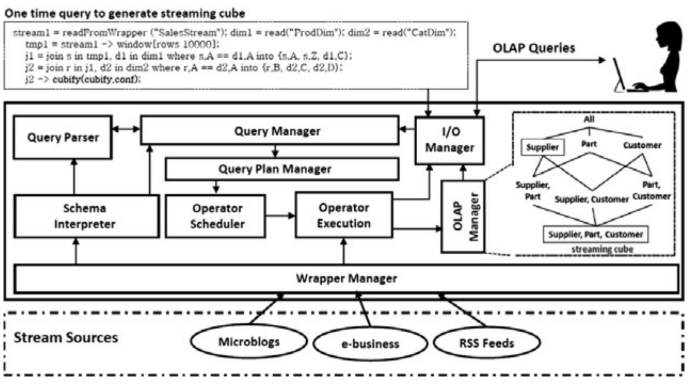

Figure 11 Stream OLAP Architecture

Approximate OLAP on Sustained Data Streams

To enable real-time OLAP analysis over data streams, the data to be analyzed must reside on memory, however due to the limited main memory size and huge data size, this is not always possible. This work proposed a novel architecture AOLAP which in addition to storing raw data streams to the secondary storage, maintains data stream's summaries in a compact memory-based data structure, piece-wise linear approximation (PLA). PLA stores data summaries corresponding to each materialized node in the OLAP cube. PLA provides approximate answers to OLAP queries however can store long data streams' summaries in a comparatively smaller space.

StreamingCube: A Unified Framework for Stream Processing and OLAP Analysis

Traditionally OLAP analysis over data streams has been achieved by coupling an SPE with an OLAP engine. Coupling multiple systems is not an efficient solution as it results in lower performance, resource wastage and increased complexity and maintenance cost. To this end, we presented StreamingCube, a unified framework for data stream processing and its interactive OLAP analysis. The proposed framework possesses all the essential operators to process data streams and introduces a new operator, cubify, to maintain OLAP lattice nodes (materialized views) incrementally. The novelty of the introduced cubify operator lies in the incremental maintenance of the materialized views.

(1-3) Sequence Data Analysis

Optimization of Row Pattern Matching over Sequence Data in Spark SQL

Due to the advance of information and communications technology and sensor technology, a large quantity of sequence data (time series data, log data, etc.) is generated and processed every day. In the analysis of such sequence data, row pattern matching is essential. Row pattern matching is a method of detecting pattern occurrences in a sequence of rows. Row pattern matching for the sequence data stored in relational databases was standardized as SQL/RPR in 2016. In SQL/RPR, the user uses MATCH_RECOGNIZE clause which defines the pattern to be extracted from the sequence. Today, in addition to relational databases, there are many frameworks for processing a large amount of data in parallel and distributed computing environments. They include MapReduce and Spark. Hive and Spark SQL enable us to code data analysis processes in SQL-like query languages. Row pattern matching is also beneficial in Hive and Spark SQL. However, the computational cost of the row pattern matching process is large and it is needed to make this process efficient.

In this study, we proposed two optimization methods to reduce the computational cost for row pattern matching process. Basic idea is to reduce the number of rows before the row pattern matching by filtering out non-relevant rows that do not contribute to the results using Filtering

Query (Figure 12). We proposed two optimization methods. One is Sequence Filtering, which filters out sequences whose rows do not satisfy the conditions in the MATCH_RECOGNIZE clause. Another is Row Filtering, which filters out rows that do not satisfy the conditions from the sequence. We focus on Spark and implemented the proposed methods for Spark SQL. Through the evaluation experiments, we proved the effectiveness of our proposed optimization.

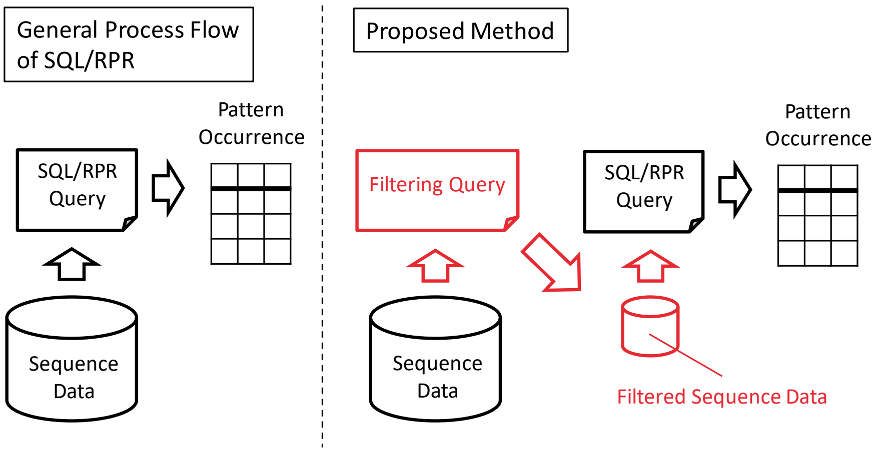

Figure 12 Filtering Out Non-Relevant Rows before Row Pattern Matching

Row Pattern Matching using Pattern Hierarchies for Sequence OLAP

Sequence OLAP is a variant of OLAP for sequence data analysis such as analysis of RFID log and person trip data. It extracts pattern occurrences of the given patterns (e.g., state transition pattern S1 → S2, movement pattern A → B) on sequence data and executes multi-dimensional aggregate using OLAP operations (such as drill-down and roll-up) and pattern OLAP operations (such as pattern-drill-down and pattern-roll-up). The pattern OLAP operations are specific to sequence OLAP and involve a hierarchy of multiple patterns. When sequence data is stored in relational databases as sequences of rows, row pattern matching finds all subsequences of rows that match a given pattern.

However, to do Sequence OLAP, especially pattern OLAP operations, on relational databases, it is required to execute row pattern matching for such a hierarchy of multiple patterns and identify parent-child relationships among pattern occurrences. Generally, row pattern matching needs a sequential scan of a large table and is an expensive operation. If row pattern matching is executed individually for each pattern, it is very time consuming. Therefore, it is strongly demanded to execute multiple row pattern matching for a given hierarchy of patterns efficiently.

Recently, SQL standard adopted a new feature called MATCH_RECOGNIZE to support row pattern matching for a single pattern. In this work, we proposed an extension of MATCH_RECOGNIZE named MULTI_MATCH_RECOGNIZE, and studied its efficient implementation. More concretely, we formalized a pattern hierarchy model for Sequence OLAP and proposed a very efficient algorithm to do multiple row pattern matching using SP-NFA (Shared Prefix Nondeterministic Finite Automaton). In experiments, we implemented our algorithm in PostgreSQL and proved the effectiveness of the proposal.

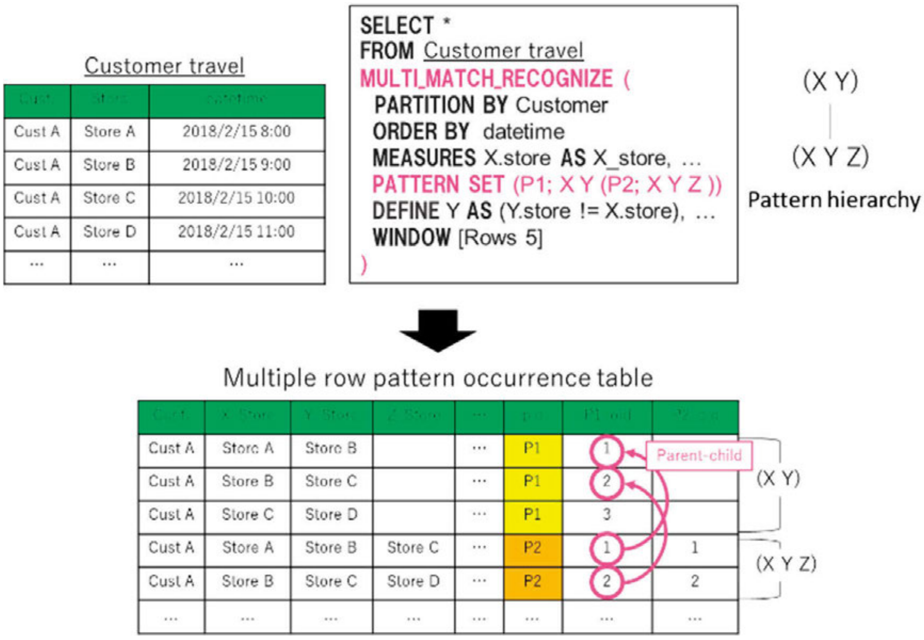

Figure 13 Row Pattern Matching using MULTI_MATCH_RECOGNIZE

(1-4) Spatial Query Processing

Dynamic Spatial-Keyword Object Search

As the popularity of SNS and GPS-equipped mobile devices rapidly grows, numerous location-based applications have emerged. A common scenario is that a large number of users change location and interests from time to time; e.g., a user watches news, blogs, and videos while moving outside. Many online services have been developed based on continuously querying spatial-keyword objects. For instance, a real-time coupon delivery system searches for potential customers using their locations and keywords of their interest, and sends coupons to attract them.

We investigated the case of dynamic spatial-keyword objects whose locations and keywords change over time. We studied the problem of continuously tracking top-k dynamic spatial-keyword objects for a given set of queries. Answering this type of queries benefit many location-aware services such as e-commerce potential customer identification, drone delivery, and self-driving stores. We developed a solution based on a grid index. To deal with the changing locations and keywords of objects, our solution first finds the set of queries whose results are affected by the change and then updates the results of these queries. We proposed a series of indexing and query processing techniques to accelerate the two procedures.

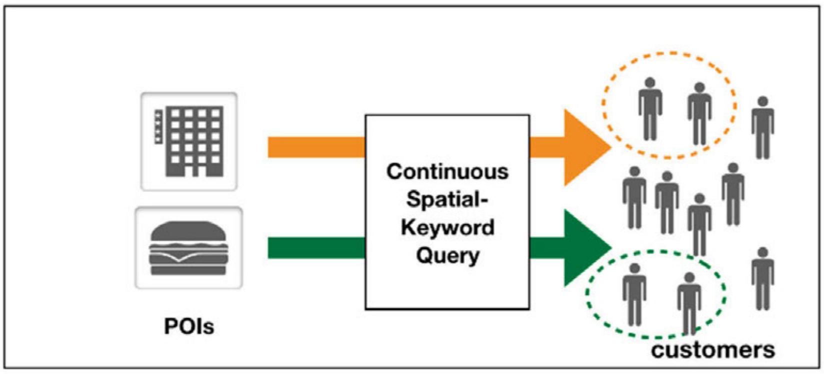

Figure 14 Dynamic Spatial-Keyword Object Search

Searching Potential Customers for Bundled Products

In the user-product mode, there are two different datasets: user preferences and products. A top-k query is a user-view common means to retrieve the top-k products for given user preference. On the other hand, the product-view methods retrieve the top-k users for a given product, which are also required from many marketing applications such as identifying potential customers for a newly released product.

Previous research for product-view methods always considers retrieving users for only one product. They cannot identify the users for a bundle with multiple products, which is an important application of a common sale strategy named "Product Bundling". To address this limitation, we proposed a new query named aggregate reverse rank query to find matching users for a set of products. To address the key challenge of high pairwise computational cost, we proposed efficient solutions with tree-based spatial indexing and branch-and-bound filtering to enhance the performance on the large user-product datasets.

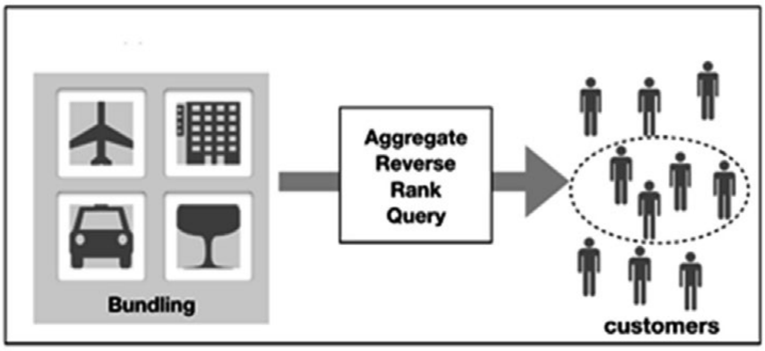

Figure 15 Searching Potential Customers for Bundled Products

2) Data Mining and Knowledge Discovery

(2-1) Outlier Detection

An outlier is an observation that deviates so much from the other observations as to arouse suspicion that it was generated by a different mechanism. Outlier detection is a key problem in data mining, and it has several applications.

Distance-based Outlier Detection on Uncertain Datasets

Uncertain data management, querying and mining have become important because most real-world data is accompanied with uncertainty these days. In this work, the uncertainty of an object is modeled with the Gaussian distribution. The Naive approach of the distance-based outlier on uncertain data is infeasible due to the expensive distance function, hence a cell-based approach was proposed, as shown in Figure 16, to enable the pruning of guaranteed inliers and to identify the outliers efficiently. Furthermore, an approximate uncertain distance-based outlier detection approach was also presented to further improve the outlier detection efficiency.

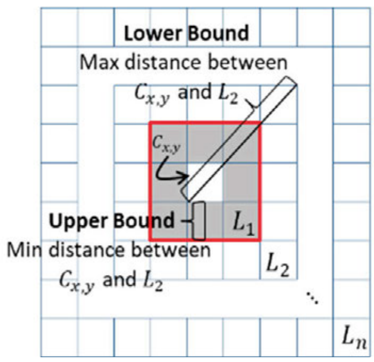

Figure 16 Cell-based Outlier Detection

Top-k Outlier Detection from Uncertain Data

This work studied the problem of top-k distance-based outlier detection from uncertain data objects. The naive approach makes use of nested loop and is expensive due to expensive distance function, hence this work proposed a populated-cells list (PC-list) approach of outlier detection capable of pruning a majority of inliers and hence can improve the top-k outlier detection efficiency. The approach makes use of the cell grid structure to identify the candidate top-k outliers as shown in Figure 17.

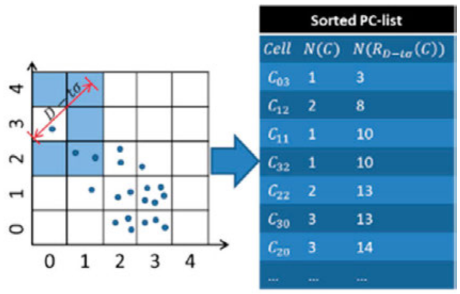

Figure 17 Top-k Outlier Detection

Continuous Outlier Detection on Uncertain Data Streams

This work studied the problem of outlier detection on uncertain time series data streams. In particular, we proposed a continuous distance-based outlier detection approach on a set of uncertain objects' states that are originated synchronously from a group of data sources (e.g., sensors in WSN). A set of objects' states at a timestamp is called a state set. Generally, the duration between two consecutive timestamps is very short and the state of all the objects may not change much in this duration. Hence, we proposed an incremental approach of outlier detection, which makes use of the results obtained from the previous state set to efficiently detect outliers in the current state set. A demo system MOOD is also developed to demonstrate the continuous outlier detection on uncertain data streams. The MOOD system provides an interface that takes moving objects' states streams and some parameters as input and continuously produces the distance-based outliers along with some graphs comparing the efficiency and accuracy of the underlying algorithms.

(2-2) Microblog and Social Media Analysis

Online Location Inference of Twitter Users

The location profiles of social media users are valuable for various applications, such as marketing and real-world analysis. As most users do not disclose their home locations, the problem of inferring home locations has been well studied in recent years. In fact, most existing methods perform batch inference using static (i.e., pre-stored) social media contents. However, social media contents are generated and delivered in real-time as social streams. In this situation, it is important to continuously update current inference results based on the newly arriving contents to improve the results over time. Moreover, it is effective for location inference to use the spatiotemporal correlation between contents and locations. The main idea of this work is that we can infer the locations of users who simultaneously post about a local event (e.g., earthquakes). Hence, in this work, we proposed an online location inference method over social streams that exploits the spatiotemporal correlation, achieving 1) continuous updates with low computational and storage costs, and 2) better inference accuracy than that of existing methods. The experimental results using a Twitter dataset show that our method reduces the inference error to less than 68% of existing methods. The results also show that the proposed method can update inference results in constant time regardless of the number of accumulated tweets.

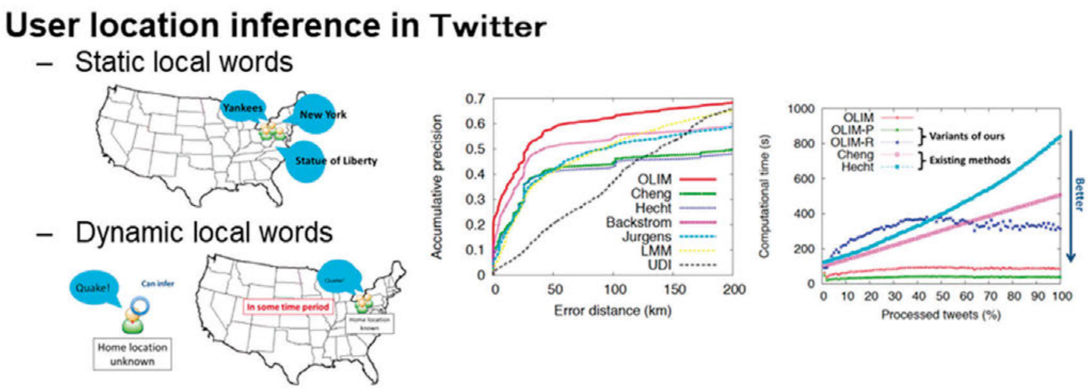

Figure 18 Online Location Inference of Twitter Users

Node Classification in Social Networks

In this work, we focused on the node classification problem on networks, which is one of the most important topics in AI and Web communities. Our proposed algorithm which is referred to as OMNIProp has the following properties: (a) seamless and accurate; it works well on any label correlations (i.e., homophily, heterophily, and mixture of them) (b) fast; it is efficient and guaranteed to converge on arbitrary graphs (c) quasi-parameter free; it has just one well-interpretable parameter with heuristic default value of 1. We also proved the theoretical connections of our algorithm to the semi-supervised learning (SSL) algorithms and to random-walks.

We also addressed the problem of exploiting confidence of the inference results. We proposed a new algorithm named CAMLP, which addresses two open challenges at the same time: (1) to handle various kinds of label correlations such as homophily and heterophily, and (2) to exploit the confidence of the inference results to enhance the accuracy. The main contributions are two-fold: (a) Novel algorithm; our algorithm is confidence-aware and is applicable to both homophily and heterophily networks, and (b) Theory; we gave theoretical analyses of our algorithm. Our experiments show that the proposed algorithm improves the precision of major competitors not only on heterophily networks, but also on homophily networks.

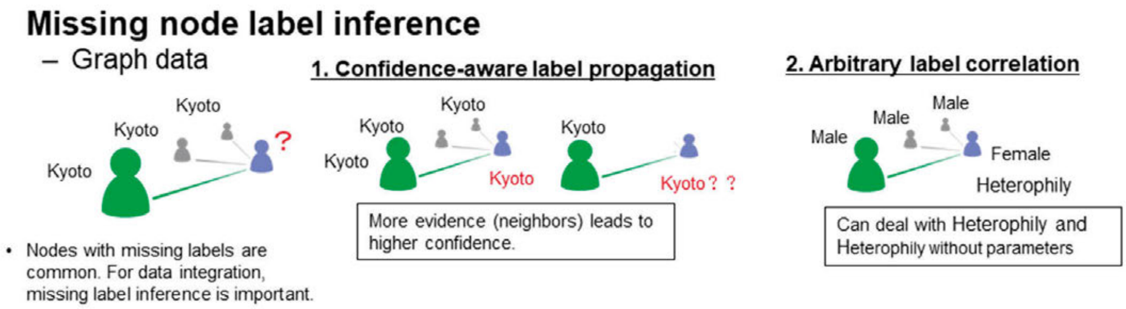

Figure 19 Node Classification in Social Networks

Collecting Non-Geotagged Local Tweets via Bandit Algorithms

We studied the problem of collecting non-geotagged tweets posted in a specific location as many as possible in a limited time span. Although there are varieties of methods to estimate the locations of users, these methods are not directly applicable to this problem because they require collecting a large number of random tweets and then filter them to obtain a small number of tweets from such users. In this research, we proposed a framework that incrementally finds such users and continuously collects tweets from them. Our framework is based on the bandit algorithm that adjusts the trade-off between exploration and exploitation, in other words, it simultaneously finds new users in the specified location and collects tweets from already-found users. The experimental results show that the bandit algorithm works well on this problem and outperforms the carefully designed baselines.

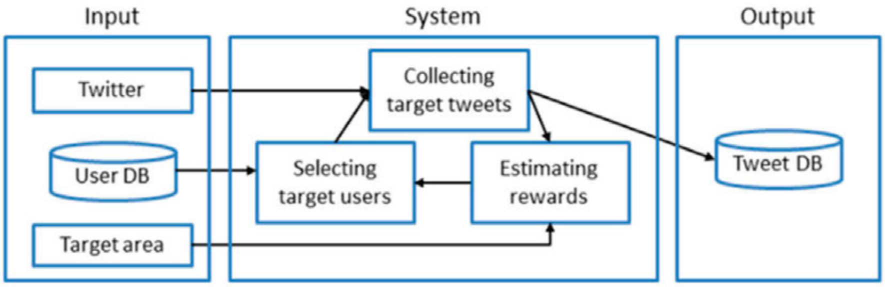

Figure 20 Collecting Non-Geotagged Local Tweets

(2-3) Graph Analysis

Graphs are now one of the most fundamental data models for representing complex entity relationships and schema-less datasets in the real world. For this reason, it is becoming increasingly important to compute large-scale graphs efficiently. To address this problem, we conducted several types of research.

ScaleSCAN: Scalable Density-based Graph Clustering

One important aspect of graphs is cluster structures where nodes in the same cluster have denser edge-connections than nodes in the different clusters. One of the most successful clustering methods is a density-based clustering algorithm called SCAN. The main concept of SCAN is that densely connected nodes should be in the same cluster; SCAN excludes nodes with sparse connections from clusters, and SCAN classifies them as either hubs or outliers. In contrast to most traditional clustering algorithms such as graph partitioning, spectral algorithm, and modularity-based method that only study the problem of the cluster detection and so ignore hubs and outliers, SCAN successfully finds not only clusters but also hubs and outliers. As a result, SCAN has been used in many applications.

Although SCAN is effective in finding highly accurate results, SCAN has a serious weakness; it requires high computational costs for large-scale graphs. This is because SCAN has to find all clusters prior to identifying hubs and outliers; it finds densely connected subgraphs as clusters. It then classifies the remaining non-clustered nodes into hubs or outliers. This clustering procedure entails exhaustive density evaluations for all adjacent node pairs included in the large-scale graphs. Furthermore, in order to evaluate the density, SCAN employs structural similarity that incurs a set intersection for each edge. Thus, SCAN requires $O(m^{1.5})$ in the worst case.

To address this issue, we developed a novel parallel-computing algorithm, ScaleSCAN, that is designed to efficiently perform on shared memory architectures with the multicore CPU. The modern multicore CPU equips a lot of physical cores on a chip, and each core highlights vector processing units (VPUs) for powerful data-parallel processing, e.g., SIMD instructions. Thus, ScaleSCAN employs a thread-parallel algorithm and data-parallel algorithm in order to fully exploit the performance of the multicore CPU. Our extensive experiments show that ScaleSCAN runs ×500 faster than SCAN without sacrificing the clustering quality. Also, ScaleSCAN achieved from ×17.3 to ×90.2 clustering speed improvements compared with the state-of-the-art algorithms. In specific, ScaleSCAN can compute graphs, which have more than 1.4 billion edges, within 6.4 s while SCAN did not finish even after 24 hours (Figure 21).

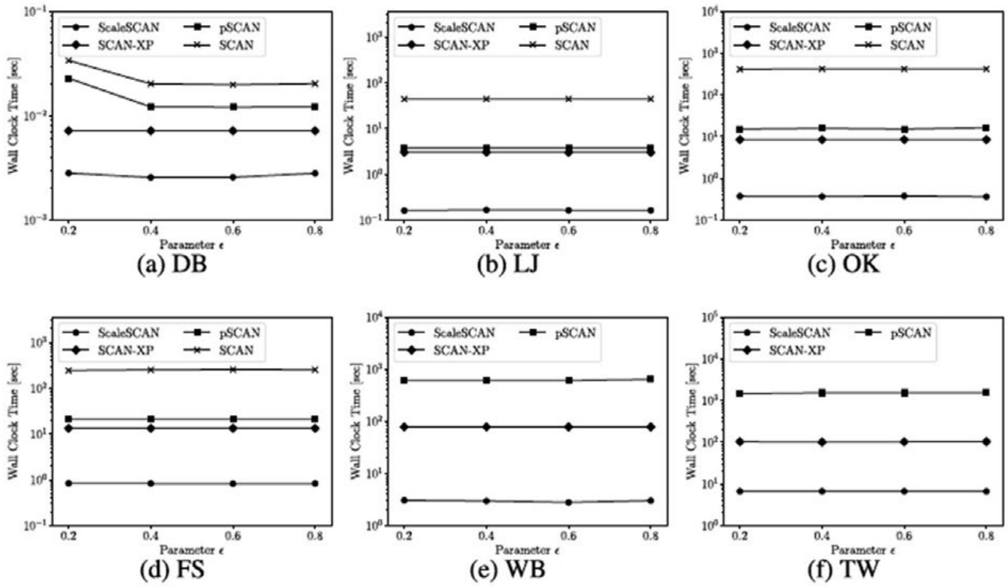

Figure 21 Running Times of ScaleSCAN on Real-World Graphs

Scaling Fine-grained Modularity Clustering for Massive Graphs

Modularity clustering is a fundamental graph analysis tool to understand complicated graphs. It detects a set of clusters that maximizes a clustering metric, modularity. Since greedily maximizing the modularity achieves better clustering results, modularity clustering is employed in various AI-based applications. Although modularity clustering is useful in many applications, it has two serious weaknesses. First, it fails to reproduce ground-truth clusters in massive graphs due to the resolution limit problem. Fortunato et al. theoretically proved that the modularity becomes larger until each cluster contains $\sqrt{m}$ edges, where m is the number of edges included in a given graph. That is, modularity maximization prefers to find coarse-grained clusters regardless of the ground-truth cluster size. Second, modularity clustering requires a large computation time to identify clusters since it exhaustively computes all nodes and edges included in a graph. In the mid-2000s, modularity clustering was applied to social networks with at most thousands of edges. By contrast, recent applications must handle massive graphs with millions or even billions of edges because graphs are becoming larger, and large graphs can be easily found.

As a result, current modularity clustering methods need to consume several dozens of hours to obtain clusters from massive graphs.

To address the above issues, we proposed a novel correlation-aware algorithm, gScarf, which is designed to handle billion-edge graphs without sacrificing the clustering quality of the original algorithm. The basic idea underlying gScarf is to dynamically remove unnecessary computations for nodes and edges from the clustering procedure. To determine which computations to exclude, gScarf focuses on the deterministic property of modularity as it is uniquely determined using only the structural properties of clusters such as degrees and cluster sizes. That is, modularity does not need to be computed repeatedly for clusters with the same structural properties. Based on the deterministic property, gScarf employs the following techniques to improve efficiency. (1) gScarf theoretically derives an incremental form of correlation-aware modularity, namely LRM-gain, (2) it introduces LRM-gain caching in order to skip unnecessary LRM-gain computations based on the deterministic property, and (3) it employs incremental subgraph folding to further improve the clustering speed. gScarf outperforms the state-of-the-art methods by up to three orders of magnitude in terms of clustering time (Figure 22). For instance, gScarf returns clusters within five minutes for a Twitter graph with 1.46 billion edges. Although modularity clustering effectively enhances application quality, it has been difficult to be applied to massive graphs. However, gScarf, which is well suited to massive graphs, should improve the quality in a wider range of AI-based applications.

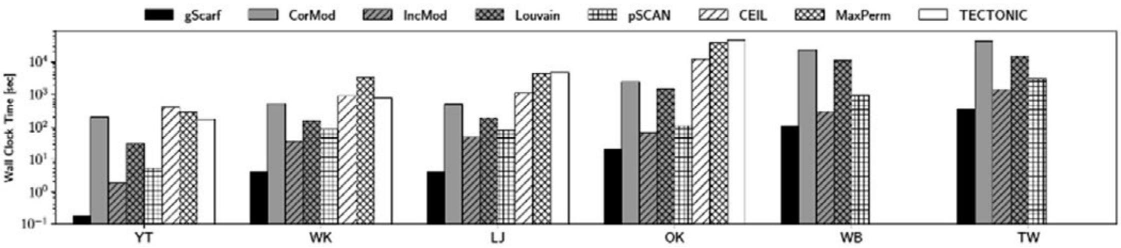

Figure 22 Running Times of gScarf on Real-World Graphs

Rabbit Order: Just-in-time Parallel Reordering for Fast Graph Analysis

In response to the emergence of billion-edge real-world graphs, massively parallel graph processing has attracted significant attention in recent years. However, parallel graph processing in HPC environments generally suffers from low scalability since graphs yield poor locality of memory accesses, which results from unstructured and complex relationships among entities represented by graphs. To improve the locality, graph reordering algorithms have been receiving increasing interests from various HPC applications. Given a graph, the graph reordering algorithms simultaneously optimize (i) computation ordering and (ii) data layout of the graph so that the graph mitigates the poor locality of memory accesses during parallel computations. The algorithms are effective in reducing cache misses incurred by the parallel graph processing. However, existing reordering algorithms still suffer from high CPU costs to find better graph reordering results.

To address this issue, we proposed a novel graph reordering algorithm called Rabbit Order that is a just-in-time parallel reordering method. Rabbit Order achieves both (1) high locality and (2) short reordering time by employing two approaches. The first approach is the hierarchal community-based reordering, which achieves higher locality than existing algorithms. The second approach is the parallel incremental aggregation that efficiently constructs the hierarchal community-based reordering on massive graphs. We experimentally verified the effectiveness of our approaches on real-world graphs, and we clarified that Rabbit Order yields the highest locality (Figure 23) within significantly short reordering times among competitive reordering algorithms.

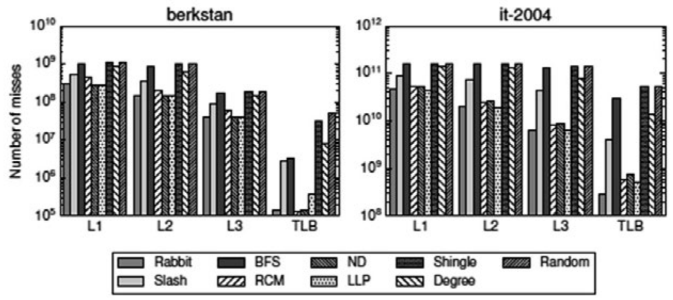

Figure 23 Number of Cache Misses and TLB Misses

(2-4) NMF and Community Detection

Non-negative matrix factorization (NMF) has been playing a fundamentally important role in analyzing various types of data in different areas of research. In our group, we have applied NMF to different tasks in big data analysis and have conducted research for improving NMF itself as well.

Detecting Topic Evolutions in Bibliographic Databases

A growing amount of academic information has been accumulated in bibliographic databases, such as DBLP DBLP, CiteSeerX, MEDLINE/PubMed, ADS, arXiv, etc., and it has become important to extract useful knowledge from those databases. To address this problem, we proposed a scheme based on NMF. Figure 16 shows an overview of the approach. More precisely, we first partition the set of publications in a database according to their publication year and apply NMF to extract clusters of publications. Notice that we take into account citation information to perform NMF for better clustering. Having obtained sets of publications for each period, we associate similar clusters in consecutive time spans according to their similarity. Thus we can obtain the time evolution of topics and clusters of publications. In the experiments, we demonstrated that the proposed scheme can successfully extract topic evolutions in real bibliographic databases, namely, CiteSeerX and arXiv.

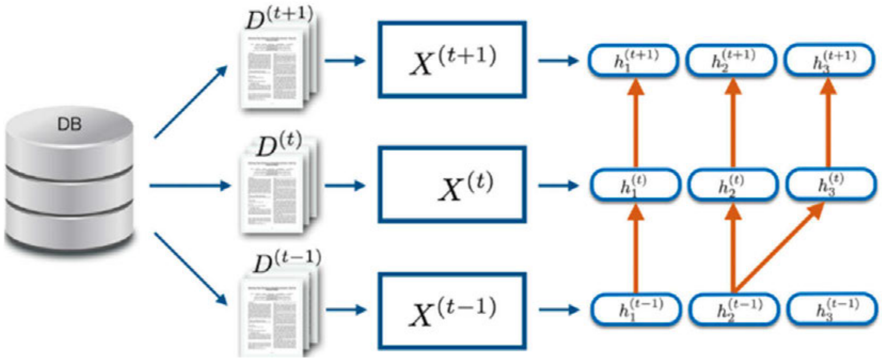

Figure 24 Detection of Topic Evolution from Bibliographic Databases

Network-word Embedding for Dynamic Text Attributed Networks

Recently, network embedding has been gaining much attention as a means to deal with network data. It allows us to map the nodes in a network into a high dimensional space while preserving the proximity of nodes as much as possible. However, few methods have been proposed as network embedding for text-attributed dynamic networks. To this problem, we proposed a novel method that embeds, for a given text-attributed dynamic network, the nodes and the words in a cooperative manner by taking advantage of temporal changes of vector representations of nodes and terms. The experimental results show that 1) vector representations of nodes of our method achieve higher accuracy than baseline methods in classification and clustering tasks; 2) the vector representations of nodes and words successfully capture semantic similarity; and 3) our method successfully captures the temporal change of the vector representations over time.

Community and Correlated Attribute Cluster Analysis on Multi-attributed Graphs

Multi-attributed graphs, in which each node is characterized by multiple types of attributes, are ubiquitous in the real world. In this study, we focused on clusters of attribute values and strong correlations between communities and attribute-value clusters. Specifically, we proposed an NMF-based algorithm that allows us to detect communities of nodes, clusters of attributes, and their relationship (CAR) at the same time. Experimental evaluation using real-world datasets shows that the proposed CARNMF can detect communities and attribute-value clusters more accurately than existing comparable methods. Furthermore, clustering results obtained using the CARNMF indicate that CARNMF can successfully detect informative communities with meaningful semantic descriptions through correlations between communities and attribute-value clusters.

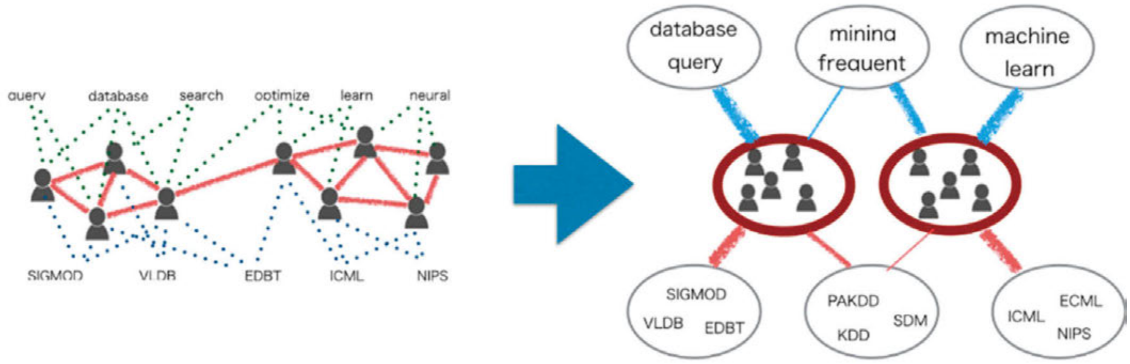

Figure 25 Detecting Node Community, Attribute Cluster, and their Relationships at the Same Time

NMF under Probabilistic Constraints

In many cases, NMF deal with probability matrices, where elements are probability values, but existing optimization algorithms do not take into account the probabilistic constraints explicitly. In this work, we proposed a novel optimization algorithm for NMF under probability constraints, thereby achieving better performance in terms of accuracy without losing efficiency. More precisely, our theoretical analysis of our algorithm shows that: 1) our method monotonically decreases the objective function; 2) the output matrices satisfy the probability constraint; 3) its learning rate is the largest while among satisfying 1) and 2); and 4) the computational time complexity remains the same as the existing optimization method. We conducted experimental evaluations using a real-world dataset by applying the proposed method to different tasks. The results show that, when applying it to topic modeling, the accuracy of clustering and topic detection is better than the ordinary NMF. When applying it to an algorithm for community detection and attribute-value clustering over multi-attributed graphs (CARNMF), it also achieved higher accuracy compared to the original NMF optimization.

(2-5) Data Analysis using GPU and FPGA

GPU (graphics processing unit) has been playing an essential role not only in processing graphics but also in the area of high-performance computing, big data processing, and artificial intelligence (AI) workloads. Besides, FPGA (field-programmable gate array) has been gaining growing attention as a device to enhance the performance in different types of workloads, such as stream processing, big data processing, and AI workloads. To extend the applicability and the performance of GPU and FPGA, we have conducted the following research works. Due to the space limitation, we only show the main results.

Probabilistic Frequent Itemset Mining on a GPU Cluster

Probabilistic frequent itemset mining, which discovers frequent itemsets from uncertain data, has attracted much attention due to inherent uncertainty in the real world. Many algorithms have been proposed to tackle this problem, but their performance is not satisfactory because handling uncertainty incurs high processing costs. To accelerate such computation, we utilized GPUs (Graphics Processing Units). Our previous work accelerated an existing algorithm with a single GPU. In this work, we extended the work to employ multiple GPUs. Proposed methods minimize the amount of data that needs to be communicated among GPUs, and achieve load balancing as well. Based on the methods, we also presented algorithms on a GPU cluster. Experiments show that the single-node methods realize near-linear speedups, and the methods on a GPU cluster of eight nodes achieve up to a 7.1 times speedup.

GPU-accelerated Canopy Clustering

Canopy clustering is a preprocessing method for standard clustering algorithms such as k-means and hierarchical agglomerative clustering (Figure 18). Canopy clustering can significantly reduce the computational cost of clustering algorithms. However, canopy clustering itself may also take a vast amount of time for handling massive data, if we naïvely implement it. To address this problem, we presented efficient algorithms and implementations of canopy clustering on GPUs, which have evolved recently as general-purpose many-core processors. We did not only accelerate the computation of original canopy clustering, but also proposed an algorithm using grid index. This algorithm partitions the data into cells to reduce redundant computations and, at the same time, to exploit the parallelism of GPUs. Experiments show that the proposed implementations on the GPU are two times faster on average than multi-threaded, SIMD implementations on two octa-core CPUs.

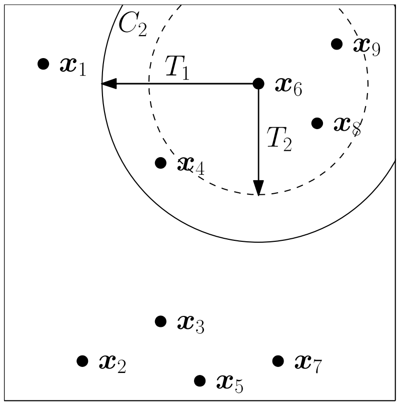

Figure 26 Canopy Clustering

GPU Acceleration of Set Similarity Joins

Due to the rapid growth and diversification of data, there is an increasing demand for fast execution of set similarity joins in applications that vary from data integration to plagiarism detection. To tackle this problem, our solution takes advantage of the massive parallel processing offered by GPUs. Additionally, we employed MinHash to estimate the similarity between two sets in terms of Jaccard similarity. By exploiting the high parallelism of GPUs and the space efficiency provided by MinHash, we can achieve high performance without sacrificing accuracy. Experimental results show that our proposed method is more than two orders of magnitude faster than the serial version of CPU implementation, and 25 times faster than the parallel version of

CPU implementation while generating highly precise query results.

GPU-accelerated Graph Clustering via Parallel Label Propagation

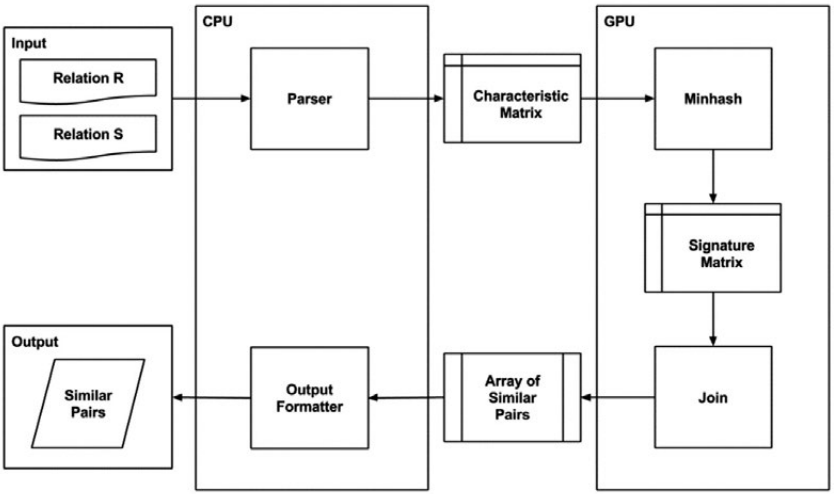

Figure 27 Set-Similarity Join on GPU

Graph clustering has recently attracted much attention as a technique to extract community structures from various kinds of graph data. Since available graph data becomes increasingly large, the acceleration of graph clustering is an important issue for handling large-scale graphs. To this end, this work proposed a fast graph clustering method using GPUs. The proposed method is based on parallelization of label propagation, one of the fastest graph clustering algorithms. Our method has the following three characteristics: (1) efficient parallelization: the algorithm of label propagation is transformed into a sequence of data-parallel primitives; (2) load balancing: the method takes into account load balancing by adopting the primitives that make the load among threads and blocks well balanced; and (3) out-of-core processing: we also developed algorithms to efficiently deal with large-scale datasets that do not fit into GPU memory. Moreover, this GPU out-of-core algorithm was extended to simultaneously exploit both CPUs and GPUs for further performance gain. Extensive experiments with real-world and synthetic datasets show that our proposed method outperforms an existing parallel CPU implementation by a factor of up to 14.3 without sacrificing accuracy.

Accelerating Regular Path Queries using FPGA

Graphs are quite useful to represent various types of relationships among different entities and have been used in diverse fields, such as social networking analysis, linked open data (LOD), and bioscience. RPQs are queries to retrieve pairs of vertices that are reachable through a path whose labels conform to a user-specified regular expression. Despite its importance and usefulness, RPQs have not been paid much attention. In this work, we attempted to accelerate such queries using an FPGA (field-programmable gate array). Specifically, we proposed a pipelined process of RPQs by dividing a query into multiple stages (Figure 28), thereby taking advantage of pipeline parallelism. Experimental evaluations show that the proposed accelerator achieves up to 23.6x faster for the small dataset and up to 4.61x faster for large datasets than the comparative method running on CPU.

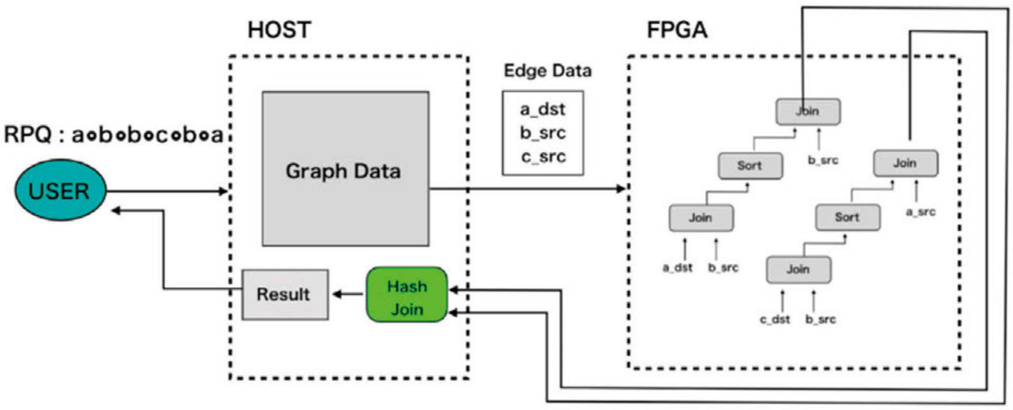

Figure 28 Processing RPQs using FPGA

Other Results

In addition, we studied the following topics: 1) GPU acceleration of similarity search for uncertain time series, 2) Efficient sort on GPUs based on data partitioning and cooperative merge, 3) Efficient position estimation based on GPU-accelerated content-based image retrieval, and 4) Approximate set similarity join using many-core processors.

3) XML, Open Data, Privacy

The volume of non-traditional data has been growing exponentially. Among others, semi-structured data, such as XML, RDF, and graph, have been used ubiquitously in a wide variety of application domains. Besides, the importance of data privacy is growing rapidly due to the demand for utilizing big data containing personal data. To address these problems, in our group, we have conducted the following research topics.

(3-1) XML Streams

Compared with query languages, keyword search has some clear benefits for its simplicity and its user-friendliness in querying XML databases. Therefore, a great deal of effort has been put on this search paradigm by trying to improve the quality of search results of pure keyword search, where only keywords are allowed as a query. However, due to the vagueness of keyword search, it is hard to accurately express real search intention with just keyword search. We observe that there are many cases where the combination of path-based query and keyword search is a better choice and can deal with such a challenge. To address this problem, we proposed a method to integrate XPath and keyword search so that users can accurately express their search demands. The idea is to convert the query expression into NFA and process XML stream using it (Figure 29). The experimental results show that the proposed scheme can process queries over XML streams practically.

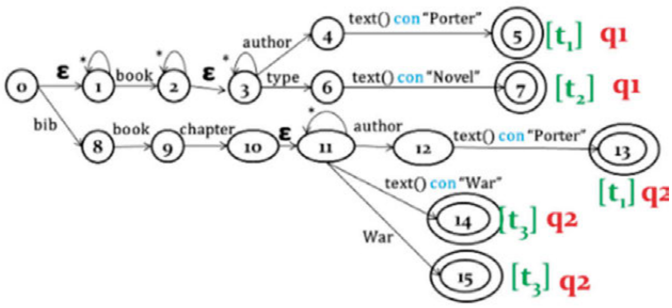

Figure 29 NFA for XPath with Keywords

(3-2) Facet Search

Faceted search is a type of user interface where multi-attribute objects are classified according to a set of facets, and users can browse those objects by choosing facets and values of their interest. It has been applied in many interfaces in different problem domains. However, applying it to semi-structured data or unstructured data is not trivial due to structural flexibility. We have studied methods to apply the faceted search to semi-structured data.

Automated Object and Facet Extraction for Faceted Search over XML Data

This work proposed an automatic extraction scheme of objects and facets from XML data for subsequent faceted search over the XML data. We proposed two approaches, namely, a frequency-based approach and a semantic-based approach, and also a hybrid approach of them. The basic ideas of these approaches are that the frequently occurring XML elements seem to be objects and facets, and such XML elements may have a semantically meaningful name. Although the proposed approaches are rather simple, the experiments using real-world XML data show that the proposed approaches can automatically extract objects and facets from the XML data.

Frequent-pattern Based Facet Extraction from Graph Data

Graph is being used in a wide variety of application domains to represent different types of data. However, querying graphs is not easy. Faceted search is a promising approach to reduce the burden of searching graph data. Applying faceted search for graph data requires to determine objects (target sub graphs) and facets. To achieve this, in this work, we proposed a framework for faceted search over graph data. The framework is organized into two phases, namely, extraction phase and search phase. The main objective of this work is to develop the extraction phase which has two main tasks, one is to extract target sub graphs, and the other is to extract facets. We apply frequent sub graph mining techniques to extract target sub graphs and facets. The proposed framework is experimentally evaluated using publicly available graph datasets, namely, citation network data and review network data, which shows the proposed framework works as expected.

(3-3) RDF, Knowledge Base, LOD

Linked Open Data (LOD) is becoming a standardized means to publish data on the Internet and is used to represent various kinds of data and knowledge bases. We have studied methods for querying or analyzing such data.

A System for Querying RDF Data using LINQ

We proposed a system that allows users to query RDF data without learning SPARQL. Instead, we introduced a JSON-style view on top of SPARQL endpoints. Having defined JSON-style views, ordinary users can issue queries against the views using LINQ, a structured query language similar to SQL. The system translates LINQ queries to corresponding SPARQL queries according to the view definition and sends the translated query to the SPARQL endpoint. The resulting data returned by SPARQL endpoints are processed and returned to the user. We conducted experiments to show the feasibility of the proposed system.

SPARQL-based ETL Framework for OLAP over Linked Data

This work proposed a framework called SPOOL that streamlines the ETL (extract, transform, and load) of LOD for subsequent OLAP analysis over numerical data contained in the data. Typically, users need to get the whole dataset to extract the necessary data. Instead, SPOOL allows users to do it without downloading the whole datasets. SPOOL provides series of SPARQL queries extracting objects and attributes from LD datasets, and converts them into star/snowflake schemas, and materialize relevant triples as fact and dimension tables for OLAP. The applicability of SPOOL is evaluated using exiting LD datasets on the Web, and SPOOL successfully processes the LOD datasets to ETL for OLAP.

ObjectRank-based Keyword Search over Linked Data

This work proposed a keyword search method that ranks entities in linked data (LD) according to the ranking score calculated by ObjectRank, a well-known link-structure analysis algorithm that can deal with heterogeneous graphs. One of the challenges is how to set appropriate edge weights in the authority transfer schema graph, which regulates the importance of different node types in the graph. FORK involves a relevance feedback algorithm to modify the authority transfer weights according to users' relevance judgments for ranking results. The experimental evaluation of ranking qualities using an entity search benchmark showcases the effectiveness of FORK, and it proves ObjectRank is a more feasible raking method for LD search than PageRank and other comparative baselines, including information retrieval techniques and graph analytic methods.

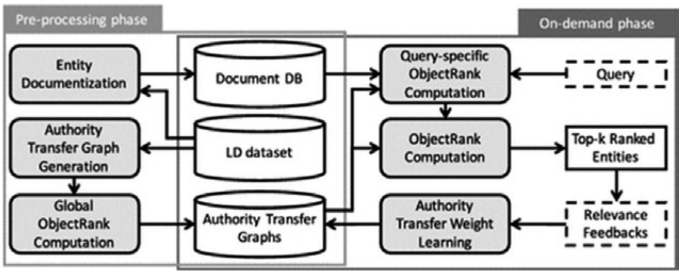

Figure 30 FORK System Overview

A Modular Approach for Efficient Simple Question Answering over Knowledge Base

We proposed an approach for efficient question answering (QA) of simple queries over a knowledge base (KB), whereby a single triple consisting of (subject, predicate, object) is retrieved from a KB for a given natural language query. More precisely, instead of constructing the end-to-end complex neural network, our method decomposes the task in a three step-pipeline: entity detection, entity linking and relation prediction. Our proposed approach is quite simple but performs reasonably well compared to previous complex approaches. We introduced a novel index that relies on the relation type to filter out subject entities from the candidate list so that the object entity with the highest score becomes the answer to the question. Furthermore, due to its simplicity, our approach can significantly reduce the training time compared to other comparative approaches. The experiment on the SimpleQuestions data set finds that basic LSTMs, GRUs, and non-neural network techniques achieve reasonable performance while providing an opportunity to understand the problem structure.

(3-4) Privacy and Anonymization

Data privacy has become one of the major concerns in the big data and AI systems. To enhance data privacy, we have studied the following topics.

A Scheme for Fast k-concealment Anonymization

In this research, we devised an improved algorithm for k-concealment, which has been proposed as an alternative to the well-known k-anonymity model. k-concealment achieves similar privacy goals as k-anonymity; it proposes to generalize records in a table in such a way that each record is indistinguishable from at least k-1 other records, while achieving higher utility than k-anonymity. However, its computation is quite expensive in particular when dealing with large datasets containing massive records due to its high computational complexity. To cope with this problem, we proposed neighbor lists, where for each record, similar records are stored. Neighbor lists are constructed in advance, and can also be efficiently constructed by mapping each record to a point in a high-dimensional space and using appropriate multidimensional indexes. Our proposed scheme successfully decreases the execution time from O(kn2) to O(k2n+knlogn), and it can be practically applied to databases with millions of records. The experimental evaluation using a real dataset reveals that the proposed scheme can achieve the same level of utility as k-concealment while maintaining the efficiency at the same time.

An Index-based Secure Query Processing Scheme for Outsourced Databases

Due to the rapid proliferation of cloud computing services in diverse applications, such as database as a service (DBaaS), encrypted database systems (EDBSs) have been gaining much attention as a way to construct secure databases in DBaaS. However, most of the existing works suffer from poor performance when dealing with large data. Some works proposed index-based query processing schemes, but they have a privacy problem that the order of attribute values may be revealed from the index structure on the server. To address this problem, we proposed a novel secure index-based query processing scheme, where the order of attribute values is not disclosed. In the scheme, the index is maintained in such a way that the structural information regarding the index and the values (or index entries) are maintained separately, and only the latter is stored in a cloud server. When searching, a client uses the structural information (without entries) to traverse the index by cooperating with cloud servers, thereby securing the order among the index entries. We prove that, in our scheme, the order among the index entries would not be disclosed even though the data and the query log are disclosed. In addition, our experimental results show that the proposed scheme significantly outperforms existing state-of-the-art schemes.

Secure Similarity Joins using Fully Homomorphic Encryption

Similarity joins are important database operations that can identify pairs of roughly similar records. Due to their many applications (e.g., duplicate elimination and plagiarism detection), a number of algorithms have been created to enhance similarity joins, especially in terms of performance. However, in some cases, the privacy of the data being joined also becomes an important aspect to consider, as leaking sensitive information can result in grave consequences for individuals, enterprises, and governmental organizations. We proposed a protocol for secure execution of similarity joins that is based on fully homomorphic cryptosystems, which are resistant to a number of attacks and provide flexibility to calculate the similarity between encrypted records. We also considered the adaptation of filter techniques to improve the efficiency of the protocol by reducing the number of record pairs that are compared. In addition, we exploited modern hardware to parallelize the solution and evaluated the performance of the proposal using real datasets.

Other Results

In addition to the above results, we conducted the following research works: 1) privacy-preserving ontology mapping, 2) label-bag based graph anonymization via edge addition, 3) a k-anonymization algorithm on social network data that reduces distances between nodes, 4) privacy-preserving record linkage with record-wise linkage policy, and 5) privacy-preserving pre-consensus protocol for blockchains.

4) Database Applications and Data Science

(4-1) Sleep Medical Science

Automated Sleep Stage Scoring for Mice

The sleep of mice consists of three stages: wake, non-REM, and REM. Identifying the sleep stage of mice from their biological signals ("sleep stage scoring") is an essential inspection in sleep research. However, this inspection is very time-consuming and requires much expertise.

To enhance the efficiency of sleep research, several automated methods for sleep stage scoring have been proposed; however, these methods have not achieved the required accuracy in sleep research. Notably, they cannot handle noisy signals. In this research, we collaborated with International Institute for Integrative Sleep Medicine (IIIS) and developed novel methods for sleep stage scoring.

“MASC,” which is the scoring method we first proposed, consists of a Fast Fourier Transform (FFT) and a support vector machine. This model achieved a high accuracy of more than 95%; however, its robustness against noise is not enough for practical use. Various kinds of noise are included in the biological signal that the FFT modules could not separate all of them in the scoring procedure.

To tackle this problem, we developed another scoring method, "MC-SleepNet," using deep learning technology. This model employs the convolutional neural network that can automatically locate the useful features for sleep stage scoring. Although it requires a vast amount of training samples, we could prepare enough sleep records of more than 4000 mice, thanks to IIIS.

The evaluation experiments show that MC-SleepNet achieves an accuracy of more than 96.7%. Besides, its accuracy does not decrease even in the case that the input signals contain much noise (Figure 31).

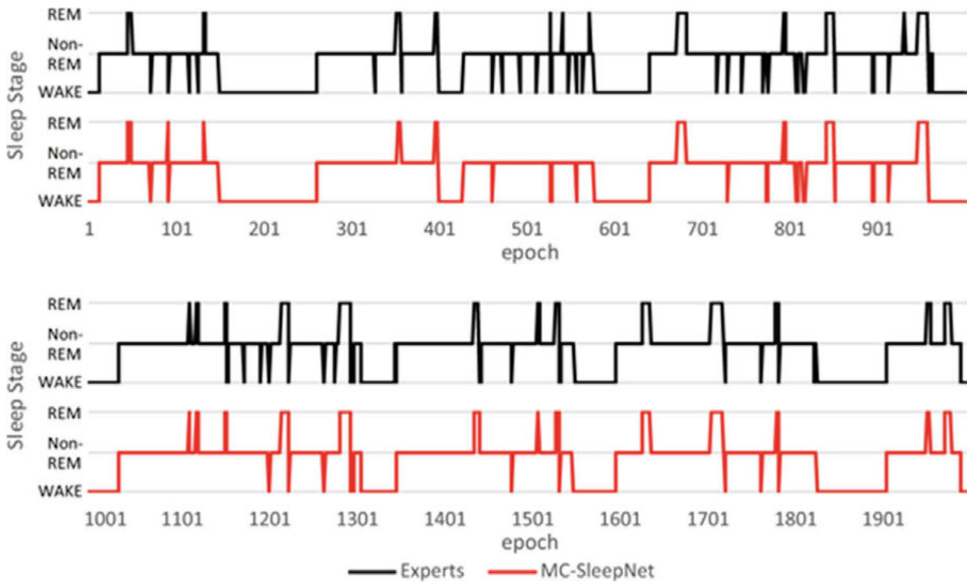

Figure 31 Sleep Stage Scoring using MC-SleepNet

Noise Reduction for Biological Signals

Moreover, we developed a deep learning model for reducing noise in biological signals. The existing noise reduction model requires the pair of noisy signals and their clear signal parts for training; however, it is tough to prepare these pairs in the case of biological signals.

In this research, we focused on generative adversarial networks (GANs), which do not require the pair of input/output signals in their training procedure, and improved its structure and learning protocols to be suitable for reducing noise in the biological signals. The proposed model, "NR-GAN," achieved the performance at the same level as the optimized frequency filters without any knowledge about noises.

(4-2) Biodata Science

As a part of our interdisciplinary collaboration with other divisions at CCS, we have been collaborating with the Molecular Evolution Group in the Division of Life Sciences. Also, we have been conducting collaborative research with a group in the Graduate School of Life and Environmental Sciences.

System for Phylogenetic Analyses over Alignments of Next Generation Sequence Data

A large quantity of DNA sequence data is being generated at high speed and at low cost by next-generation sequencing (NGS) technology in recent years. NGS influences a wide range of biology, including evolutionary biology, which is the field that infers the evolutionary relationships of genes or organisms from sequence data. In particular, the phylogenetic analyses using a massive amount of data generated by NGS have been actively conducted. To infer the phylogenetic relationship, a number of alignments that comprise sets of sequences need to be maintained, i.e., they need to be updated whenever new sequence data become available. However, there has been no database that supports updates of alignments, i.e., addition and/or removal of sequences from existing alignments. Instead, individual researchers independently update their alignments manually. To cope with this problem, we proposed a system for phylogenetic analyses over alignments of NGS data. It takes as input NGS data, predicts the orthologue that each sequence belongs to, and updates the alignments. Moreover, by describing the related alignments in a tree structure, it can maintain stored alignments in a systematic way. To prove the concept, we implemented a prototype web application. We expect that our system helps biological researchers carry out phylogenetic analysis on large scale data, including those from NGS.

Prediction of Mitochondrial/Mitochondrion-related Organelle Proteins of Nonmodel Organisms

To estimate the functions of mitochondria of diverse eukaryotic nonmodel organisms in which the mitochondrial proteomes are not available, it is necessary to predict the protein sequence features of the mitochondrial proteins computationally. Various prediction methods are trained using the proteins of model organisms belonging particularly to animals, plants, and fungi exist. However, such methods may not be suitable for predicting the proteins derived from nonmodel organisms because the sequence features of the mitochondrial proteins of diversified nonmodel organisms can differ from those of model organisms that are present only in restricted parts of the tree of eukaryotes. Here, we proposed NommPred, which predicts the mitochondrial proteins of nonmodel organisms that are widely distributed over eukaryotes. We used a gradient boosting machine to develop two predictors: one for predicting the proteins of mitochondria and the other for predicting the proteins of mitochondrion-related organelles that are highly reduced mitochondria. The performance of both predictors was found to be better than that of the best method available.

Predicting the Decision Making Chemicals Used for Bacterial Growth

Predicting the contribution of media components to bacterial growth was first initiated by introducing machine learning to high-throughput growth assays. A total of 1336 temporal growth records corresponding to 225 different media, which were composed of 13 chemical components, were generated. The growth rate and saturated density of each growth curve were automatically calculated with the newly developed data processing program. To identify the decision making factors related to growth among the 13 chemicals, big datasets linking the growth parameters to the chemical combinations were subjected to decision tree learning. The results showed that the only carbon source, glucose, determined bacterial growth, but it was not the first priority. Instead, the top decision making chemicals in relation to the growth rate and saturated density were ammonium and ferric ions, respectively.

(4-3) Smart City

Analyzing and feeding back the results on real-world services are important missions in the Big Data era to realize smart city. Feasibility for obtaining data acceleratingly increases demands for data analysis. For instance, sensing devices, social networking services, etc. provide data like sensed data such as temperature, humidity, textual posts and so on. Such data are really useful for improving qualities in real-world services. For example, when a traffic jam is observed from road-sensing as well as users' posts on social networking services, navigation applications can give suggestions to drivers heading to the area of the jam. Analyzing real-world data is still challenging because of the following reasons: dirtiness of data and a large variety of analytic requirements. Data with carefully designed schema are highly useful and easy to analyze, however, real-world services tend to have poorly designed schema since they are aimed to just record but not to analyze. Data with poor schema for analyses require data cleansing such as noise elimination, schema reconstruction, consistency checking, and so on. Furthermore, combining multiple real-world dirty data is bothersome. In addition, analytical scenarios for recorded data are not always clear because data are not designed for analyses. It is often the case that supplemental information or knowledge based on human experiences are required for the analytical scenarios.

To cope with the challenges for analyzing smart city data, we developed an overall toolbox (Figure 32) for analyzing real-world data. The toolbox is composed of three phases: (1) preparation phase, (2) analysis phase, and (3) visualization phase. The toolbox accepts not

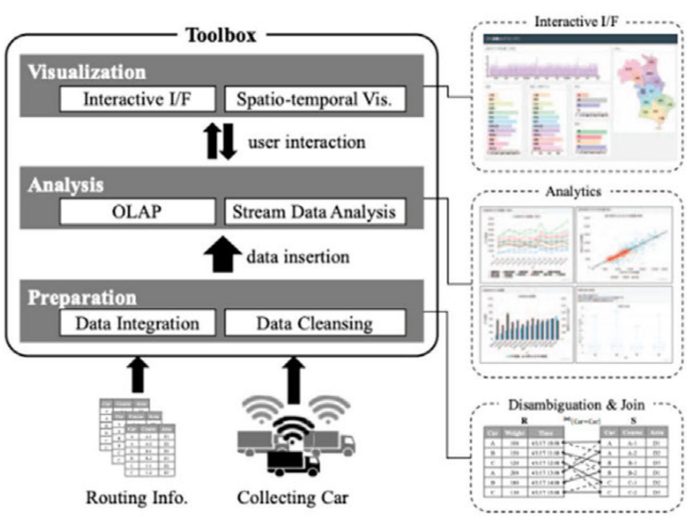

Figure 32 Developed Analytical Toolbox for Smart City

only static records but also streaming data. The preparation phase deals with the dirtiness of real-world data by providing data integration (e.g., joining inconsistent data) and data cleansing techniques (e.g., noise elimination). The analysis phase provides OLAP and streaming OLAP as analytical processing on the cleaned data, since OLAP functionalities can support a large variety of analytical requirements for ordinary applications. The analysis phase supports OLAP analysis as well as streaming data analysis. The visualization phase is capable of showcasing the analytical results with interactive interfaces as well as spatio-temporal visualization.

We assessed the applicability and capability of the toolbox through the use case of a garbage collection log analysis scenario. The garbage collection log consists of garbage amounts from all over Fujisawa city, Japan, and it is highly reliable to obtain knowledge and facts of the civic tendency for garbage. The analytical scenario is that the city attempts to reduce the amount of garbage from the city, because collecting and treating the garbage takes high costs. To approach this problem, the application aims to motivate citizens by providing information about how a large amount of garbage in their lives and promoting competitive incentives to reduce the garbage amounts comparing with other blocks of the city. To do so, the application reveals the amount of garbage from citizens in various perspectives.

(4-4) Posture Analysis

Humans spend on average more than half of their day sitting down. The ill-effects of poor sitting posture and prolonged sitting on physical and mental health have been extensively studied, and solutions for curbing this sedentary epidemic have received special attention in recent years. With the recent advances in sensing technologies and Artificial Intelligence (AI), sitting posture monitoring and correction is one of the key problems to address for enhancing human well-being using AI. We presented the application of a sitting posture training smart cushion called LifeChair that combines a novel pressure sensing technology, a smartphone app interface and machine learning (ML) for real-time sitting posture recognition and seated stretching guidance. We presented our experimental design for sitting posture and stretch pose data collection using our posture training system. We achieved an accuracy of 98.93% in detecting more than 13 different

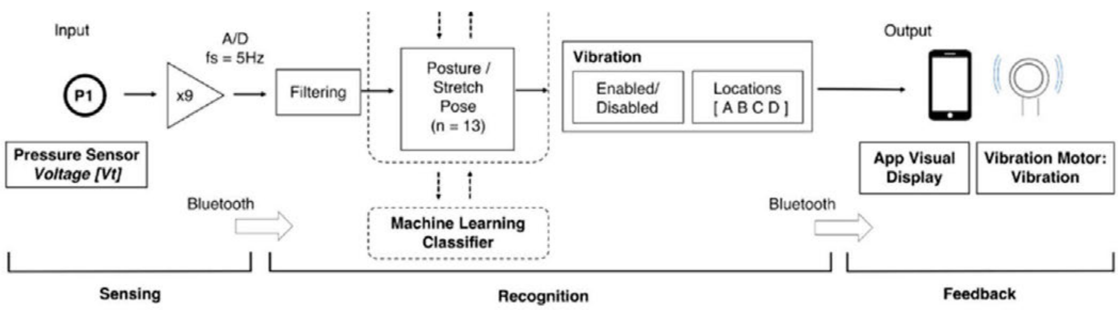

Figure 33 Posture Analysis System Overview

sitting postures using a fast and robust supervised learning algorithm. We also identified the importance of taking into account the divergence in user body mass index in posture monitoring. Additionally, we presented the first ML-based human stretch pose recognition system for pressure sensor data and how its performance in classifying six common chair-bound stretches.

9.3 Collaboration

Division of Global Environmental Science

By collaborating with Division of Global Environmental Science and the Division of High Performance Computing Systems, we have been contributing to developing and maintaining GPV/JMA Archive and JRA-55 Archive, which are Web-based public database service to archive meteorological data released from the Japan Meteorological Agency (JMA). GPV/JMA Archive services six kinds of data, including global spectral model data (GSM), regional spectral model data (RSM), meso-scale non-hydrostatic model data (MSM), weekly ensemble forecast data, monthly ensemble forecast data, and seasonal ensemble forecast data. Meanwhile, JRA-55 Archive serves the state-of-the-art long-term reanalysis of global weather data in grid point values (GPV).

Division of Particle Physics

We have been contributing to the management of JLDG (Japan Lattice Data Grid), which is a scientific data grid for sharing lattice QCD gauge configuration data in computational particle physics, as well as ILDG (International Lattice Data Grid). More precisely, we have been mainly in charge of managing ILDG-related services, such as the metadata server and faceted search interface. For the last four years, we have been working on assigning DOI (Digital Object Identifier) to the public QCD ensembles. To this end, CCS has become a member of JalC (Japan Link Center), which is the management body of DOI in Japan. Now, we have been working on the system at CCS.

International Institute for Integrative Sleep Medicine (IIIS)

In collaboration with International Institute for Integrative Sleep Medicine (IIIS), University of Tsukuba, we have been working on big sleep data analysis. The theme of big sleep data analytics and automatic sleep diagnosis is one of the major research topics in the Computation Medical Science project. Our group is strongly committed to this research topic. Sleep plays an important role in people's daily lives. Sleep disorders could cause various illnesses. Actually, there are a lot of scientific questions that need to be answered about sleep. Quantitative and accurate measurements and analysis of sleep are fundamental issues in sleep research. Sleep polysomnography (PSG) is a commonly used sleep measurement method. However, in PSG, the burden and cost of the subject are large, and measurement over a long period is impossible. Moreover, analysis of the acquired data depends on manual inspection by human experts, and it is impossible to analyze large-scale data. In response to the increasing social interest in sleep in recent years, some methods have been developed to easily measure sleep status using a smartphone or the like. However, at present, there is still no means to measure sleep conveniently as accurately as human experts. This research aims to realize automatic sleep analysis and diagnosis by integrating sleep big data analysis, machine learning and new sensing technology, and to pioneer a new computational medical science field.

Other Collaborations

Besides, we have been collaborating with 1) the Research Unit 3 in the R & D Division at JAXA (Japan Aerospace Exploratory Agency) in extracting useful knowledge from various documents, including specifications and failure reports and 2) Prof. Ouchi at ICRR, the University of Tokyo in applying Deep-Neural Networks to automatically detect galactic images of specific types out of massive images captured by HSC (Hyper Supreme-Cam) of Subaru Telescope.

9.4 Future Plan

Research and Development for Data Engineering Challenges

Big data is tightly combined with machine learning and AI technologies, and has been giving huge impacts on many aspects of human life and society. To address the technical issues and challenges involved in big data, we have studied a wide variety of topics in data engineering. Especially, we have conducted our research from the viewpoints of (1) information integration framework, (2) data mining and knowledge discovery, and (3) XML, open data, and privacy. We will continue to perform research and development in those areas intensively. In particular, big data involves many aspects such as Volume, Variety, Velocity, Veracity, and others. In our research, we will try to continue addressing all these aspects of our research.

Use of Powerful Computing Facilities for Big Data Analysis

Recently, the use of powerful computing facilities for big data challenges has been attracting much attention. CCS has powerful computing facilities such as Cygnus and Oakforest-PACS. We have worked hard on parallel data processing and use of GPU, many cores, and FPGA for big data analysis, and proved their effectiveness through different research topics. There are a lot of research issues remaining in this area. We will also try to make our research results beneficial for users to utilize Cygnus and Oakforest-PACS for big data analysis.

Scientific Data Management

One of the essential missions of our group is to contribute to managing and utilizing scientific data. With this in our mind, we have been working with different scientific data: meteorological data (GPV/JMA Archive and JRA-55 Archive), Lattice QCD data (JLDG and ILDG), sleep big data, biological data, etc. We will continue and further extend our activity to other partners in different areas of research.

Contribution to Computational Medical Science

The theme of big sleep data analytics and automatic sleep diagnosis is one of the major research topics in the Computation Medical Science project in CCS. Our group is strongly committed to this research topic. We have been strongly collaborating with International Institute for Integrative Sleep Medicine (IIIS), University of Tsukuba in this project. There are a lot of scientific questions that need to be answered about sleep. We hope that our collaborative research results will contribute to sleep medical science and our society.

Reinforcement of Cooperation with Other Divisions and Organizations

So far, we have collaborated with the Division of Global Environmental Science, the Division of High Performance Computing Systems, the Division of Particle Physics, and the Division of Life Sciences in CCS. We will continue the ongoing collaboration points and will further expand collaborations with other divisions if any opportunity arises.

Regarding the collaboration with organizations outside of CCS, we have collaborated with International Institute for Integrative Sleep Medicine (IIIS) and the Research Unit 3 in the R & D Division in Japan Aerospace Exploration Agency (JAXA). We have also collaborated with many industrial partners in research on stream processing and data mining. We will continue our endeavor to return our research contributions to society.

9.5 Publications

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26th - 29th 2019.

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Books

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Awards

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2. iiWAS2015 Best Paper Award: Takahiro Komamizu, Toshiyuki Amagasa, and Hiroyuki Kitagawa, "SPOOL: A SPARQL-based ETL Framework for OLAP over Linked Data", Proc. 17th International Conference on Information Integration and Web-based Applications & Services (iiWAS 2015), pp. 351-360, Brussels, Belgium, December 11-13, 2015.
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4. 2016 年度電子情報通信学会優秀論文賞: 藤原 靖宏, 中辻 真, 塩川 浩昭, 三島 健, 鬼塚 真, "Personalized PageRank に対するアドホックな検索手法", 電子情報通信学会論文誌, Vol. J98-D, No. 5, pp. 774-787, May 2015.
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6. DEXA 2016 Best Paper Award: Yuyang Dong, Hanxiong Chen, Kazutaka Furuse, and Hiroyuki Kitagawa, "Aggregate Reverse Rank Queries", Proc. 27th International Conference on Database and Expert Systems Applications (DEXA 2016), pp. 87-101, Porto, Portugal, September 5-8, 2016.
7. ICDIM 2017 Best Paper Award: Chihiro Sakazume, Hiroyuki Kitagawa, Toshiyuki Amagasa, "DIO: Efficient Interactive Outlier Analysis over Dynamic Datasets", Proc. 12th International Conference on Digital Information Management (ICDIM 2017), pp. 234-241, Fukuoka, Japan, September 12-14, 2017.
8. WebDB Forum 2017 論文賞: 藤森 俊匡, 塩川 浩昭, 鬼塚 真, "分散グラフ処理におけるグラフ分割", WebDB Forum 2017.
9. DEIM 2018 最優秀インタラクティブ賞: 長城 沙樹, 北川 博之, "時系列文書に対する効率的なエンティティリンキング", 第 10 回データ工学と情報マネジメントに関するフォーラム (DEIM 2018) , C1-6, 2018 年 3 月 4 日～3 月 6 日.
10. DEIM 2018 優秀インタラクティブ賞: 伊藤 寛祥, 駒水 孝裕, 天笠 俊之, 北川 博之, "ノードがテキスト情報を持つ動的ネットワークにおけるノードと単語の分散表現学習", 第 10 回データ工学と情報マネジメントに関するフォーラム (DEIM

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11. DEIM 2018 優秀論文賞: 佐藤 朋紀，塩川 浩昭，北川 博之, "選択的重要度先読みを用いた ObjectRank の高速化", 第 10 回データ工学と情報マネジメントに関するフォーラム (DEIM 2018) , I7-5, 2018 年 3 月 4 日～3 月 6 日.
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13. BigComp 2019 Best Paper Award Runner-up: Hiroyoshi Ito, Toshiyuki Amagasa, "An Optimization Scheme for Non-negative Matrix Factorization under Probability Constraints", Proc. 6th IEEE International Conference on Big Data and Smart Computing (BigComp 2019), Kyoto, Japan, February 27th - March 2nd, 2019.
14. DEIM 2019 優秀インタラクティブ賞: 安坂 祐紀, 渡辺 知恵美, 天笠 俊之, 北川博之, "取引額を秘匿したブロックチェーンにおける取引者間合意による資産売買プロトコル", 第 11 回データ工学と情報マネジメントに関するフォーラム (DEIM 2019) , I6-4, 2019 年 3 月 4 日～3 月 6 日.
15. ICBSP 2019 Best Presentation Award: Yuki Sumiya, Kazumasa Horie, Hiroaki Shiokawa, Hiroyuki Kitagawa, "NR-GAN: Noise Reduction GAN for Mice Electroencephalogram Signals", Proc. 4th International Conference on Biomedical Imaging, Signal Processing (ICBSP 2019), Nagoya, Japan, October 17-19 2019.
16. 情報処理学会コンピュータサイエンス領域功績賞：北川博之, 2019 年 10 月.

9.6 Grants

1. JSPS/Grant-in-Aid for Scientific Research (B): 日本学術振興会/科学研究費助成事業：基盤研究(B)「複合型並列計算環境を活用した大模不均質データの実時間分析基盤」（2014-2016）(研究代表者 北川博之)，17,160,000 円
2. JSPS/Grant-in-Aid for Scientific Research (C): 日本学術振興会/科学研究費助成事業：基盤研究(C)「EPUB3.0 を核とした知識集積型ソーシャルリーディング基盤に関する研究」（2013-2015）(研究代表者 天笠俊之)，4,680,000 円
3. JSPS/Grant-in-Aid for Scientific Research (A): 日本学術振興会/科学研究費助成事業：基盤研究(A)「大規模・異種の時空間データ統合で生じる矛盾を許容するサイエンスクラウド基盤」（2012-2014）（研究代表者 小島功）（研究分担者　北川博之，天笠俊之），1,365,000 円
4. MEXT/Research and Development on Real World Big Data Integration and Analysis: 文部

科学省/国家課題対応型研究開発推進事業：未来社会実現のための ICT 基盤技術の研究開発「ビッグデータ利活用のための研究開発」(2014-2015)（研究代表者　北川博之），2014 年度 36,675,000 円， 2015 年度 37,341,000 円

5. Commissioned Research: 受託研究「時系列データベース・分析技術の研究開発」(2014)（研究代表者　北川博之），500,000 円
6. Commissioned Research: 受託研究「時系列データの分析基盤技術の研究」(2014)（研究代表者　北川博之），2,000,000 円
7. JSPS/Grant-in-Aid for Scientific Research on Innovative Areas: 日本学術振興会/科学研究費助成事業：新学術領域研究「超ストレス環境・宇宙を見据えた新規睡眠覚醒制御手法の開発」（2015-2019）(研究代表者　長瀬博)（研究分担者　北川博之），10,500,000 円
8. JSPS/Grant-in-Aid for Scientific Research (A):日本学術振興会/科学研究費助成事業：基盤研究（A)「災害後の復旧・復興における共有情報管理のための基盤技術に関する研究」(2013-2016) (研究代表者　横田治夫)（研究分担者　天笠俊之），1,250,000 万円
9. Commissioned Research: 受託研究「安心安全なデータの管理および活用に関する研究」(2015)（研究代表者　北川博之），1,080,000 円
10. Commissioned Research: 受託研究「機械学習の適用によるログ及び資産情報からの例外的状況の自動検出」(2015)（研究代表者　北川博之），5,000,000 円
11. Joint Research: 共同研究「Twitter のユーザー分析」(2015)(研究代表者　北川博之), 550,000 円
12. Commissioned Research: 受託研究「時系列データの分析基盤技術の研究」(2015)（研究代表者　北川博之），2,000,000 円
13. JSPS/Grant-in-Aid for Research Activity Start-up: 日本学術振興会/科学研究費助成事業：科学研究費研究活動スタート支援「大規模グラフの頻出部分構造を利用した高速な分析アルゴリズムの開発」(2016-2017)(研究代表者　塩川浩昭), 2,990,000 円
14. RIKEN/Research and Development on Real World Big Data Integration and Analysis: 国立研究開発法人理化学研究所/試験研究「実社会ビッグデータ利活用のためのデータ統合･解析技術の研究開発」(2016-2017)(研究代表者　北川博之)2016 年度 32,967,000 円，2017 年度 33,777,000 円
15. NICT/BigClouT Project: 独立行政法人情報通信研究機構（NICT）/欧州との連携による公共ビッグデータの利活用基盤に関する研究開発「スマートシティにおける市民の影響力を拡張するビッグデータ・クラウド・IoT 融合基盤技術」(2016-2019) (研究代表者　NTT 東日本)（研究分担者　北川博之），2016 年度 8,250,000 円，2017 年度 10,250,000 円，2018 年度 8,663,411 円，2019 年度 3,250,000 万円

16. MEXT/Program for Building Regional Innovation Ecosystems: 文部科学省/地域イノベーション・エコシステム形成プログラム「つくばイノベーション・エコシステムの構築（医療・先進技術シーズを用いた超スマート社会の創成事業）」(2016-2019))（研究代表者 TGI）(研究分担者　北川博之), 2016 年度 15,000,000 円, 2017 年度 15,000,000 円，2018 年度 10,289,001 円，2019 年度 10,230,000 円
17. Commissioned Research: 受託研究「機械学習の適用によるログ及び資産情報からの例外的状況の自動検出」(2016)（研究代表者　北川博之），3,000,000 円
18. Commissioned Research: 受託研究「多様なデータ統合・活用のための基盤技術」(2016)（研究代表者　北川博之），2,000,000 円
19. JST/Strategic Basic Research Program ACT-I: 科学技術振興機構/戦略的創造研究推進事業 ACT-I 「Data Skewness を捉えた超高速・省メモリな大規模データ処理」(2017-2018）(研究代表者　塩川浩昭)，3,900,000 円
20. 国立研究開発法人日本医療研究開発機構 : 臨床研究等 ICT 基盤構築研究事業「エビデンスの飛躍的創出を可能とする超高速・超学際次世代 NDB データ研究基盤構築に関する研究」(2017)（研究代表者　満武巨裕）(研究分担者　北川博之), 6,760,000 円
21. Joint Research: 共同研究「複合イベント処理や機械学習などの技術を利用し、ログ及び資産情報から警告すべき状況の高速かつ柔軟な検出を実現する」(2017)（研究代表者　北川博之），3,330,000 円
22. Joint Research: 共同研究「脳波、筋電データの深層学習に関する研究」(2017)（研究代表者　北川博之），2,200,000 円
23. Commissioned Research: 受託研究 :「多様なデータ統合・活用のための基盤技術」(2017)（研究代表者　北川博之），2,000,000 円
24. JSPS/Grant-in-Aid for Early-Career Scientists: 日本学術振興会/科学研究費助成事業 : 若手研究「超並列計算環境における大規模グラフの実時間問合せ処理」(2018-2020)(研究代表者　塩川浩昭)，4,160,000 円
25. 厚生労働省/厚生労働行政推進調査補助金 : 政策科学総合研究事業（政策科学推進研究事業）「ナショナルデータベース（NDB）データ分析における病名決定ロジック作成のための研究」(2018)（研究代表者　満武巨裕）(研究分担者　北川博之), 3,000,000 円
26. Joint Research: 共同研究「データエンジニアリングの知見の応用によるログ及び資産情報の処理の高速化・軽量化・高度化」(2018)（研究代表者　北川博之），330,000 円
27. 奨学寄附金「データ工学を中心とする次世代情報化社会の基盤システムの研究」(2018)(共同研究代表者　天笠俊之，北川博之，塩川浩昭)，1,000,000 円

28. Cross-ministerial Strategic Innovation Promotion Program: 内閣府/戦略的イノベーション創造プログラム(SIP)：スマートバイオ産業・農業基盤技術「食を通じた健康システムの確立による健康寿命の延伸への貢献」(2018)（研究代表者　山本万里） (研究分担者　北川博之), 8,696,000 円
29. JSPS/Grant-in-Aid for Scientific Research (B): 日本学術振興会/科学研究費助成事業：基盤研究（B）「高水準仮想化機能をもつ Augmented リアルビッグデータ利活用基盤の構築」(2019-2022)(研究代表者　北川博之), 17,160,000 円
30. JSPS/Grant-in-Aid for Challenging Research (Exploratory): 日本学術振興会/科学研究費助成事業；挑戦的研究（萌芽）「深層学習による個人特性を反映した生体データの自動生成」（2019-2020）(研究代表者　北川博之), 6,370,000 円
31. JSPS/Grant-in-Aid for Early-Career Scientists: 日本学術振興会/科学研究費助成事業：若手研究「敵対的生成ネットワークを用いたノイズ除去手法の開発と生体信号への応用」(2019-2021)(研究代表者　堀江和正), 4,290,000 円
32. JST/Strategic Basic Research Program ACT-I: 科学技術振興機構/戦略的創造研究推進事業 ACT-I 加速フェーズ「Data Skewness を捉えた超高速・省メモリな大規模データ処理」（2019-2020）(研究代表者　塩川浩昭),　2019 年度 13,000,000 円
33. Joint Research: 共同研究「データエンジニアリングの知見の応用によるログ及び資産情報の処理の高速化・軽量化・高度化」(2019)（研究代表者　北川博之）, 3,330,000 円
34. JST/Mirai Program: 科学技術振興機構/未来社会創造事業：食・運動・睡眠等日常行動の作用機序解明に基づくセルフマネジメント「睡眠脳波を指標とする睡眠と運動の自己管理による健康寿命延伸」(2019-2020) （研究代表者　柳沢正史）（研究分担者　北川博之）, 2019 年度 1,300,000 円

10 Division of Computational Informatics: Computational Media Group

10.1 Overview

The Computational Informatics Research Division is founded in 2004, and the medium-term/long-term mission of this division is to investigate novel methods at the frontier of computational informatics through computational media, which will be a crucial technology to unite human beings and vast data/high-performance computation world.

Since computational media should be used as a tool to promote collaboration between people and data/processes at the computer side, real-time processing, and instant reaction are essential. We call this research framework, “Real-World Computational Informatics.”

As for the computer-side resources, sensors, databases, grid/cloud computing, and computer network should be integrated gracefully. They should be served in a fashion of fusion of data and process to users as a form of computational media. Cameras and their videos are the primary resources in our group because we think visional communication is the most promising path to let people understand the digital world intuitively and deeply. We utilize Virtual Reality, Augmented Reality, and Mixed Reality for this purpose.

Our research achievements have been published to leading international journals in the areas of computer vision and virtual reality. We have been promoting collaboration with many application fields that covers the medication, assistive technology, sports analysis, sports training support, world heritage preservation, industries like mining, etc.

The members of the group are Prof. Yoshinari Kameda, Prof. Itaru Kitahara, and Assistant Professor Hidehiko Shishido. Our research activities have been supported partially from the research funds listed here. Since we have many funds, only the most related funds in 2014-2019 are listed. We appreciate their support. (The funded budget shows its total amount.)

10.2 Research Results

Since our research activities cover many research literature and application fields, eleven specific issues among them are shown here.

1) Visual Exploratory Activity for Read-The-Game Skill Evaluation of Football Players and for Behavioral Analysis under Microgravity Conditions

Visual Exploratory Activity is one of the key issues to investigate human behavior in virtual space. We have been working on this issue for visual skill development both on the athlete (football player) and astronaut who should work in a microgravity environment. The same cutting edge technology opens a new vista in both applications.

[Football] This research project proposes a Virtual Reality (VR) system that allows both players and coaches to measure Active Visual Exploratory Activity patterns (AVEA). The primary purpose of the system is to analyze the ability to “read the game” of soccer players under pressure. By making use of Head Mounted Display (HMD) technology and it’s head tracking capabilities, the users experience an in-game situation. They are set in the place of a defender with ball possession before making a passing decision while being pressured by a rival player. Therefore, being forced to make quick decisions based on visual information. By extracting the motion tracking data of the HMD, the gazing direction of the user is saved and divided into three zones of interest. A trial test was carried (N=10) to evaluate the system, and the IPQ questionnaire was applied post-session for analyzing AVEA performance and present relationship.

[Microgravity Environment] This work explores the human visual exploratory activity (VEA) in a microgravity environment compared to one-G. Parabolic flights are the only way to experience microgravity without astronaut training, and the duration of each microgravity segment is less than 20 seconds. Under such unusual conditions, the test subject visually searches a virtual representation of the International Space Station located in his Field of Regard (FOR). The task was repeated in two different postural positions. Interestingly, the test subject reported a significant reduction of microgravity-related motion sickness while experiencing the VR simulation, in comparison to his previous parabolic flights without VR.

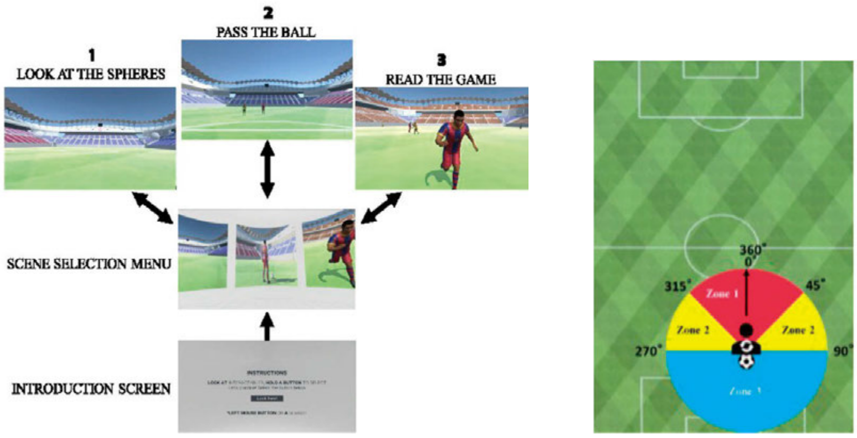

Figure 1. Experiment procedure of AVEA evaluation and the score chart for that.

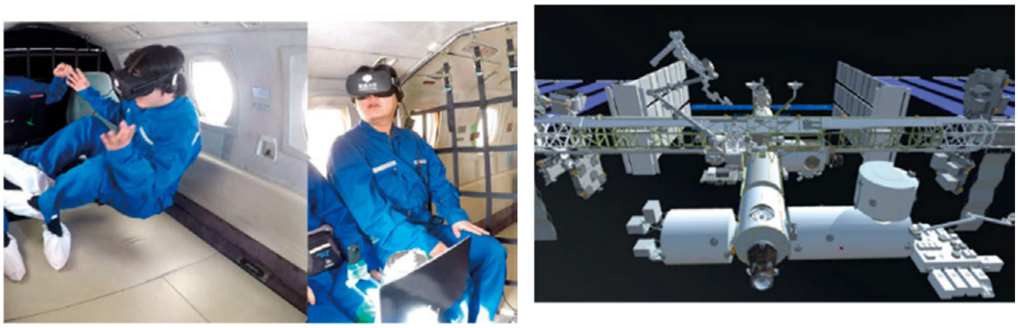

Figure 2. Snapshot of Microgravity Environnment and the target object to find in the environment.

2) Image Based Location Estimation for Walking Out of Visual Impaired Person

A new and intelligent walking navigation system could be helpful for visually impaired people so that they do not need helpers or guide dogs on going out. Conventional navigation systems using GPS are not available indoors or undergrounds. A new location estimation method that is available in such situations is necessary. We propose to estimate the pedestrian's location with only a single camera attached to the pedestrian. Our proposed method uses only computer vision, and no other sensors are needed. The location estimation is achieved by image retrieval. The retrieval database is built from a pre-recorded video taken along a planned walking path. Simple image retrieval using local image features does not work well when the images were taken in different conditions of time and weather. In this paper, we especially discuss robustness for the change of sunlight condition due to its recording time. We propose a new method of robust location estimation based on our database built by combining more than one video that is taken under different conditions. Experiment results showed that the accuracy of the location estimation using the proposed database is better than the one from a conventional database built by using a single video.

Figure 3. Correspondance of SIFT key pairs to retrieve the most similar image in the pre-recorded video. Left: Small gap in time and space. Right: Large gap in time. Our proposed method can handle these largely changing in vision.

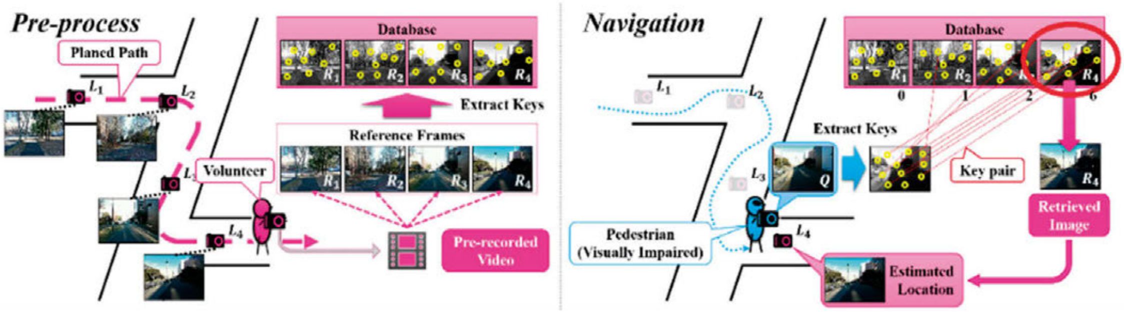

Figure 4. Location estimation procedure based on image retrieval. Left: Pre-process is done based on the pre-recorded video that is taken by a volunteer before the subject goes. Right: A subject visually impaired on his/her planned path and estimates the position by our system.

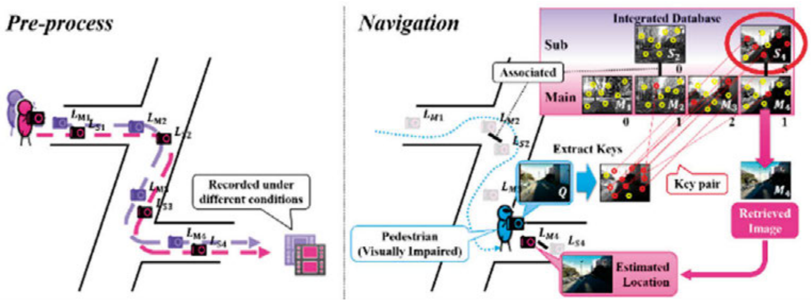

Figure 5. Technical detail of the proposed method. By utilizing two pre-recorded videos, the system can offer robust position estimation.

3) Walkable Area Estimation for Visually Impaired

When a visually impaired person has to walk out, they have to use white canes, but the range that can be scanned by a white cane is not long enough to walk safely. We propose to detect walkable plane areas on the road surface by using the RGB-D camera and the accelerometer in the tablet terminal that is attached to the RGB-D camera. Our approach can detect plane areas at a longer distance than a white cane. It is achieved by using height information from the ground and normal vectors of the surface calculated from a depth image obtained by the RGB-D camera in real-time.

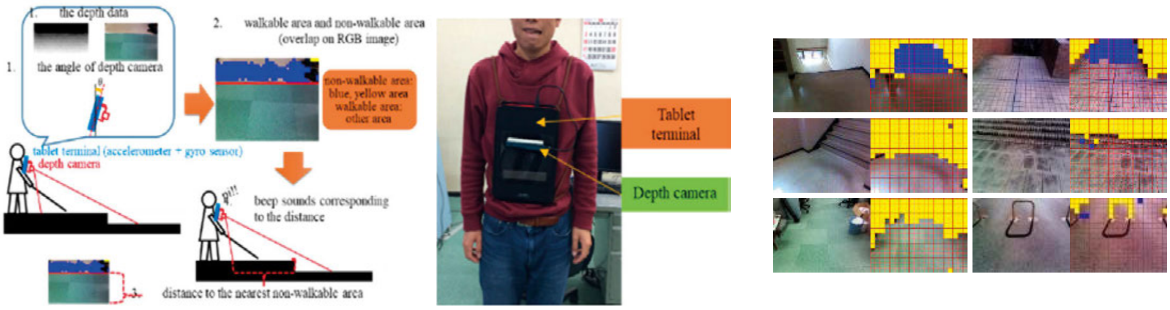

Figure 6. Detection of walkable area from depth camera image. Left: Outline of the depth image processing. Middle: A snapshot of our preliminary system. Right: 6 snpashots of the frontal view. Note that both the up(yellow) and down(blue) are detected as non-safe regions.

4) Swimmer Position Estimation by Lane Rectification

In swimming competitions, performance has been evaluated based on passing times at specific points. With this method, it is not possible to investigate the speed change based on race progress in detail. In this study, we have been conducting research on video analysis that enables detailed performance analysis along the time axis by merely installing a camera at the top of the audience seats. By this approach, it is possible to analyze swimmer information of all lanes from the swimming pool taken. In swimming, since athletes are generally near the water surface, homography conversion is performed on the swimming pool image to normalize the image to the pool surface. After that, the position of the swimmer is estimated. It is done by focusing on the color difference of the pixels in the target area. The background difference method corresponding to the events specific to swimming is also applied. With this method, we succeeded in estimating the position of each video frame.

The video of swimming games is taken from a higher seat row in the audience seat area. It can cover the whole field of a swimming pool. The swimming pool video is transformed so that each lane can be analyzed along with the lane direction. The foreground region that includes both the swimmer and their water splash is extracted by adaptive background modeling and by setting the mask region to cope with the influence of the non-planer water surface. Then, based on the color analysis on water splash, the swimmer region can be successfully extracted. The position is estimated as the center of the Gaussian distribution of the swimmer region. The proposed method was applied to a nationwide swimming game.

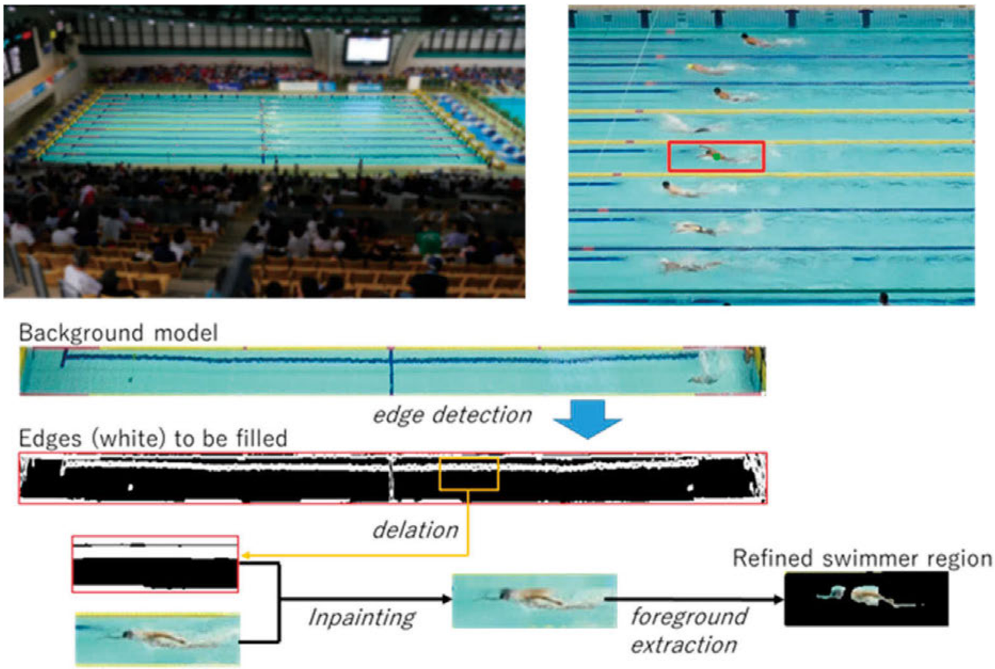

Figure 7. Swimmer position estimation for all lanes. Up-Left: whole view. Up-right: Estimated position in a lane. Bottom: Image processing procedure.

5) Multi-Resolution Bullet-Time Effect

Bullet-Time is a camera work to make the observer feel like transitioning from side to side by switching multiple-view images capturing an object. Simple switching operation realizes the Bullet-Time effect if the position and orientation of the cameras are set up so that all the optical axes intersect at a point. Practically, however, it is difficult to realize such set up in some cases. For example, setting up time is limited, or the target point is moving. It is possible to solve this problem by virtually rotating the multiple cameras so that the target point is observed at the center of all captured images. The resolution of the captured image is rapidly getting higher. When a user observes the detail of a specific region of the high-resolution image using a device having a small monitor such as a smartphone, he/she enlarges the region by using a digital zoom effect. We expect that such an operation might be used in Bullet-Time browsing, also. However, ordinal Bullet-Time has a problem. If the attention (zooming-in) point is different from the focusing point of the multi-view images, the attention object goes out of the displayed image during the switching viewpoint, as shown in the following figure (b).

We propose the Bullet-Time effect that can zooms-in the attention object with keeping a watch it, as shown in figure(c). Our proposed browser estimates the 3D position of an attention object using stereovision and makes the 3D point as a new focusing point of the multi-view images

Figure 8. (a) Original image: The green point is a focusing point of the captured multi-view images. When the user inputs a new attention point (blue one) with zooming-in, the white dotted rectangle is displayed. (b) Ordinal zoom-in Bullet-Time effect: The attended object goes out of image during switching. (c) Our proposed method: The attended object is always observed at the center of the image.

6) Smoothly Switching Method of Asynchronous Multi-view Videos Using Frame Interpolation

While the number of capturing multi-view cameras or the size of the target space becomes larger, the cost for setting becomes higher. In response to such problems, synchronous imaging methods that can be applied to large-scale spaces have been proposed by generating external synchronization signals from GPS signals and distributing them to multi-view cameras. However, such a special device makes expensive the installation cost. In order to realize reasonable image-capturing at practical shooting environments, a method synchronizing multi-view asynchronous images using audio information has been proposed. In our target environment, such as a soccer stadium, however, there is serious sounds echo effect (reflection sound), that makes difficult the synchronization process.

Moreover, if the system can archive frame-level synchronization, asynchronous of shutter-level remains since the internal clocks of the cameras are not synchronized. If we consider accurate 3D computer vision processing, completely synchronized multi-view videos taken with a huge amount of labor and specialized equipment are required. On the other hand, the bullet-time video can be generated with asynchronous videos, since it does not need accurate 3D information. However, when we capture fast-moving objects, the flickering artifact (deviations of the observed position) is observed in the bullet-time video.

We aim to reduce the deviation by using frame interpolation technique for generating bullet-time video smooth switching the viewpoint. In each multi-view video, frame interpolation processing is applied with respect to the frame before and after the frame of interest. Generally, frame interpolation processing is realized by image morphing that generates a series of image groups whose appearance changes continuously from one shape to the other using a process of synthesizing the appearance of the middle between two images. In the typical morphing method, correspondence information between two input images is manually given. However, when video data composed of 30 or more frames per second is to be processed, manually inputting required correspondence is not feasible. In order to solve this problem, we employ Regenerative Morphing that can automatically generate interpolated images even if there is no correspondence information between input images. However, when the target object moves fast, the position of the target object between the consecutive front and rear frames is significantly different. As a result, it is challenging to generate an interpolation image in which the object is clearly observed in the desired position. In this research, we deal with this problem by generating an initial interpolation image that includes the cue of visual information to generate an appropriate interpolation image from a simple correspondence.

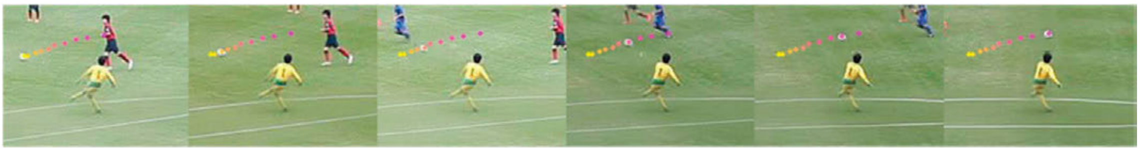

Figure 9. Perform asynchronous multi-viewpoint photographing by using an inexpensively installable capturing system in a large-scale space. In the bullet-time image using the captured image, the observation position on the image of the subject is blurred at the viewpoint switching due to the influence of the synchronization shift. Therefore, by adapting the proposed method, we generate a bullet time image in which the blur of the observation position of the object is reduced.

7) On-site Visual Feedback Method Using Bullet-Time Video

Visual feedback is attracting research attention for the development of motor learning, as it enables objective observation of the body and movement. In the common visual feedback methods, subjects observe their own body using a mirror or captured videos. Therefore, it is difficult for the subject to observe their own from various viewpoints. Observation from various viewpoints can be achieved by generating a 3D CG model of the subject using a 3D reconstruction technique or a motion capture device. However, the distortion in the synthesized 3D CG model may adversely affect the observation. To address this problem, we propose a viewport visual feedback method using multiple cameras capturing the same scene from various viewpoints. One of the technologies to effectively present a multi-view video is bullet-time video, which realizes a visual effect of a viewport moving around the subject by sequentially switching/displaying the multi-view videos along with the layout of the shooting cameras. It is possible to generate and present a high-quality image with a low processing cost, which is an important issue for visual feedback.

In order to install the bullet-time video in an on-site visual feedback system, two requirements must be satisfied. The first one is “real-time generation of bullet-time video.” On-Site visual feedback can be classified into two types: “real-time visual feedback” performed during the action and “delayed visual feedback” performed immediately after the action. Both are effective for motor learning. In the case of delayed visual feedback, the shorter the time required for feedback, the better. However, handling multi-view videos is a problem for real-time or short-time visual feedback owing to a large amount of video data. We propose a system to realize real-time/delayed visual feedback by processing all video data on a single computer to minimize the video transmission time, thereby reducing the time required for generating a bullet-time video.

The second requirement is to simplify the operation of the viewer as much as possible. For that purpose, we introduced two approaches: (a) automatic target point setting, and (b) automatic viewpoint switching. (a) Automatic target point setting: In the bullet-time video, in order to realize smooth viewpoint switching, it is necessary to adjust the direction of the shooting camera such that the optical axis of the multi-view camera crosses at one point (target point) in the capturing space. This processing is referred to as a target point setting. We realize the automation of the target point set by combining a real-time 3D sensor (RGB-D camera) and a real-time bullet-time video generation method. (b) Automatic viewpoint switching: In motor learning, when the posture of the subject at a particular moment is particularly important in the motion, we call that moment as a keyframe. By using multi-view videos, it is possible to observe keyframes from various angles. However, if the number of viewpoints is massive, it takes time to switch the viewpoint to the direction in which a keyframe is most easily and intuitively observed. In this research, by detecting keyframes, we realize the automation of viewpoint switching to the most suitable observation direction.

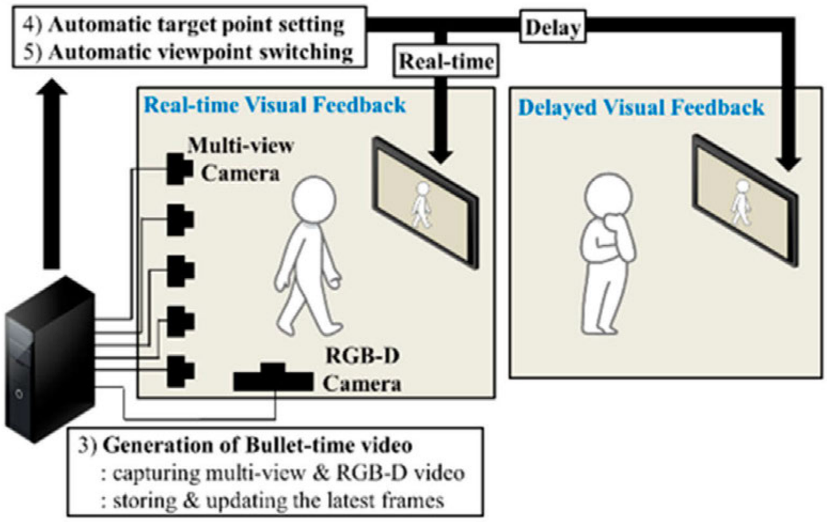

Figure 10. System overview: Multi-view video and RGB-D video are acquired with one computer. Storing and updating the latest frames for playback. Real-time visual feedback and delayed visual feedback of bullet-time video with automatic target point setting and automatic viewpoint switching is realized.

8) MR Visualization of Wheel Trajectories of Driving Vehicle by Seeing-Through Dashboard

Many efforts aim to realize a society where autonomous vehicles become general transportation in industrial, political, and academic fields. In order to make autonomous vehicles more familiar with the public, it is necessary to develop not only advanced auto-driving control but also comfortable environments for the passengers. We propose a trial to improve the comfort of passengers on autonomous vehicles. We developed an experimental vehicle equipping a Mixed Reality (MR) display system, which aims to reduce anxiety using visual factors. Our proposed system visualizes a road surface that is out of the passenger's field of view by projecting the see-through image on the dashboard. Moreover, it overlays the computer graphics of the wheel trajectories on the displayed image using MR so that the passengers can easily confirm the auto-driving control is working correctly. The displayed images enable passengers to comprehend the road condition and the expected vehicle route out of the passenger's field of view. We investigated the change of mental stress by introducing methods for measuring physiological indices, heart rate variability, and sweat information.

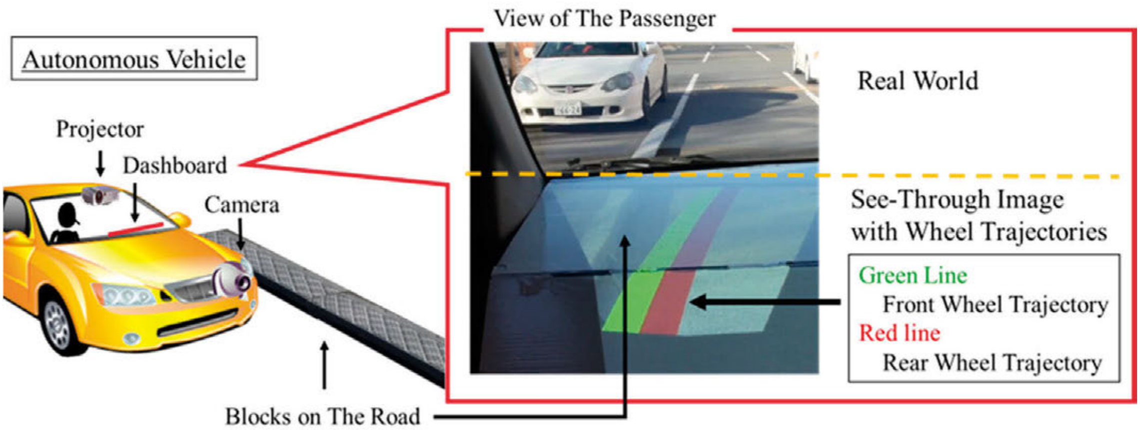

Figure 11. Our system visualizes a road surface that is out of the passenger's field of view by seeing-through the dashboard. MR visualization of wheel trajectories is realized by overlaying the CG data onto the displayed road surface.

9) A Projector Calibration Method Using a Mobile Camera for Projection Mapping System

Projection mapping systems have been used for many application fields, such as advertisements and entertainment. However, the system cannot be easily deployed by non-expert users or to an unspecialized space, thus limited the usages. The difficulty of deployment is that projector registration is always required to be carried out, and the geometry of the projection surface is required to be known to achieve the correct projection result. Many calibration methods using projector-camera systems have been proposed to simplify the process. These methods use the camera(s) to capture some projection patterns and estimate the necessary information for calibrating the projector from the correspondences between the camera and projector. However, building a projector-camera system requires the camera being installed and configured such that the projected patterns can be clearly observed, and the camera must be stationary during the calibration process. In some real-world cases, fulfilling these requirements can be difficult, and installing cameras just for system deployment is considered costly and inefficient.

The primary goal of our work is to build an easy-to-use projector calibration method to overcome the problems described above. The significant difference between the proposed method and conventional methods is that we use a mobile camera instead of one or several stationary cameras. Our method allows the users to use an inexpensive handheld camera such as a built-in camera of a smartphone to carry out projector calibration.

We propose a projector calibration method using a mobile camera and spatial coded structured light (SL). Our method allows the users to use a handheld camera to carry out projector calibration and therefore reduce the effort and time required for camera setup. Although the decoding of temporal coded SL can be error-prone in a real-world situation, our method can achieve robust calibration results by taking advantage of the multi-view observations of the projection thanks to the mobility of the camera. Experiments show that the result of our method is comparable with that of a checkerboard-based approach.

Figure 12. The structured light pattern used for calibration (left) and the experiment setup (right)

10) Calibration of multiple sparsely distributed cameras using a mobile camera

Camera calibration that estimates the projective relationship between 3D and 2D image spaces is one of the most crucial processes for such 3D image processing as 3D reconstruction and 3D tracking. A strong calibration method, which needs to place landmarks with known 3D positions, is a common technique. However, as the target space becomes large, landmark placement becomes more complicated. Although a weak-calibration method does not need known landmarks to estimate a projective transformation matrix from the correspondence information among multi-view images, the estimation precision depends on the accuracy of the correspondence. When multiple cameras are arranged sparsely, detecting corresponding sufficient points is difficult. In this project, we propose a calibration method that bridges sparse multiple cameras with mobile camera images. The mobile camera captures video images while moving among sparse multi-view cameras. The captured video resembles dense multi-view images and includes sparse multi-view images so that weak-calibration is effective. We confirmed the appropriate spacing between the images through comparative experiments of camera calibration accuracy by changing the number of bridging images and applied our proposed method to multiple capturing experiments in a large-scale space and verified its robustness.

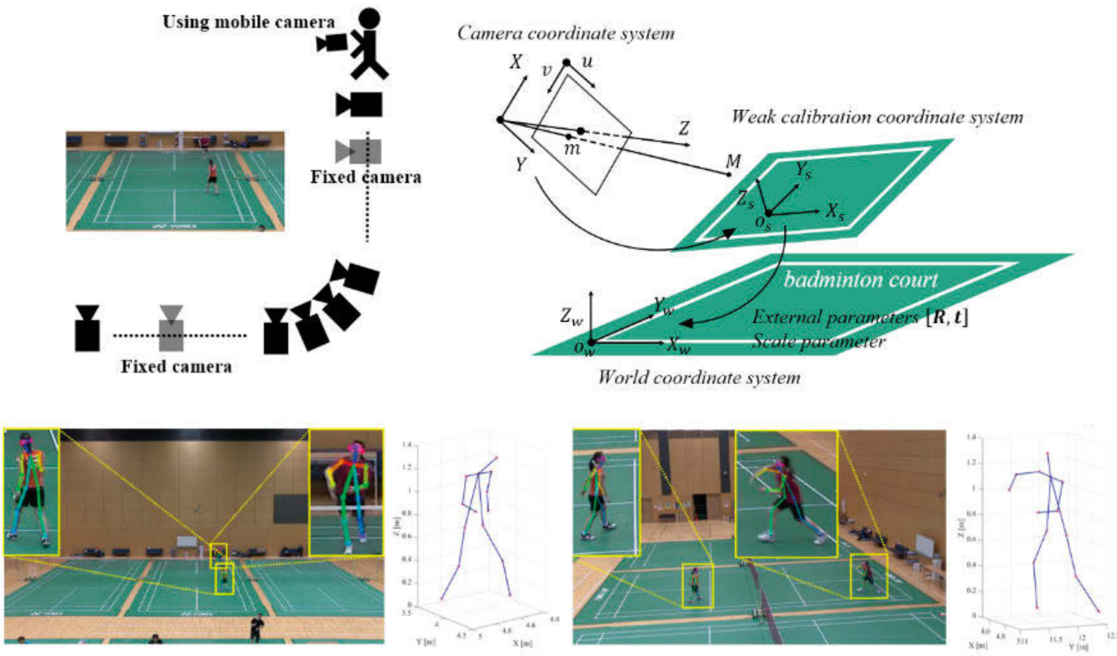

Figure 13. (Upper left) Dense images captured in our proposed method. Mobile camera captures target scene while moving among sparsely fixed multi-view cameras.
(Upper Right) Geometric relationship of camera coordinate system, weak-calibration coordinate system, and world coordinate system.
(Lower) Result of detected 2D pose and estimated 3D pose.

11) Proactive Preservation Activity of World Heritage by 3D Reconstruction Technology

In this project, a method is proposed to accurately overlap multiple high-quality images with different shooting positions and intervals by combining corresponding point information between images and 3D shape information. In the proposed method, the correct feature matching of images obtained by rendering the 3D model of the subject is used. In this project, the subjects were the pillars of the Angkor Thom Bayon Temple and the epilithic microorganisms adhering to and eroding their surfaces. Synthetic transformation of a homography utilizing the correct matches is employed to overlap the target images. When overlapping different background images using the conventional method, the estimation of the homography matrix becomes difficult owing to incorrect matches; thus, high-quality overlapping images cannot be obtained. The objective of this research was to realize the overlapping image process even under conditions that cause incorrect feature matches, such as differences in background and illumination. In this project, the damaged parts of the pillar surfaces were visualized using the proposed method. Based on the results of an experiment comparing the proposed method with an existing state-of-the-art method, the effectiveness and higher accuracy of the proposed method were verified. The findings of this research contribute to Angkor Thom Bayon Temple preservation, including a preservation project that the present authors are organizing for this culturally and historically valuable UNESCO World Heritage site.

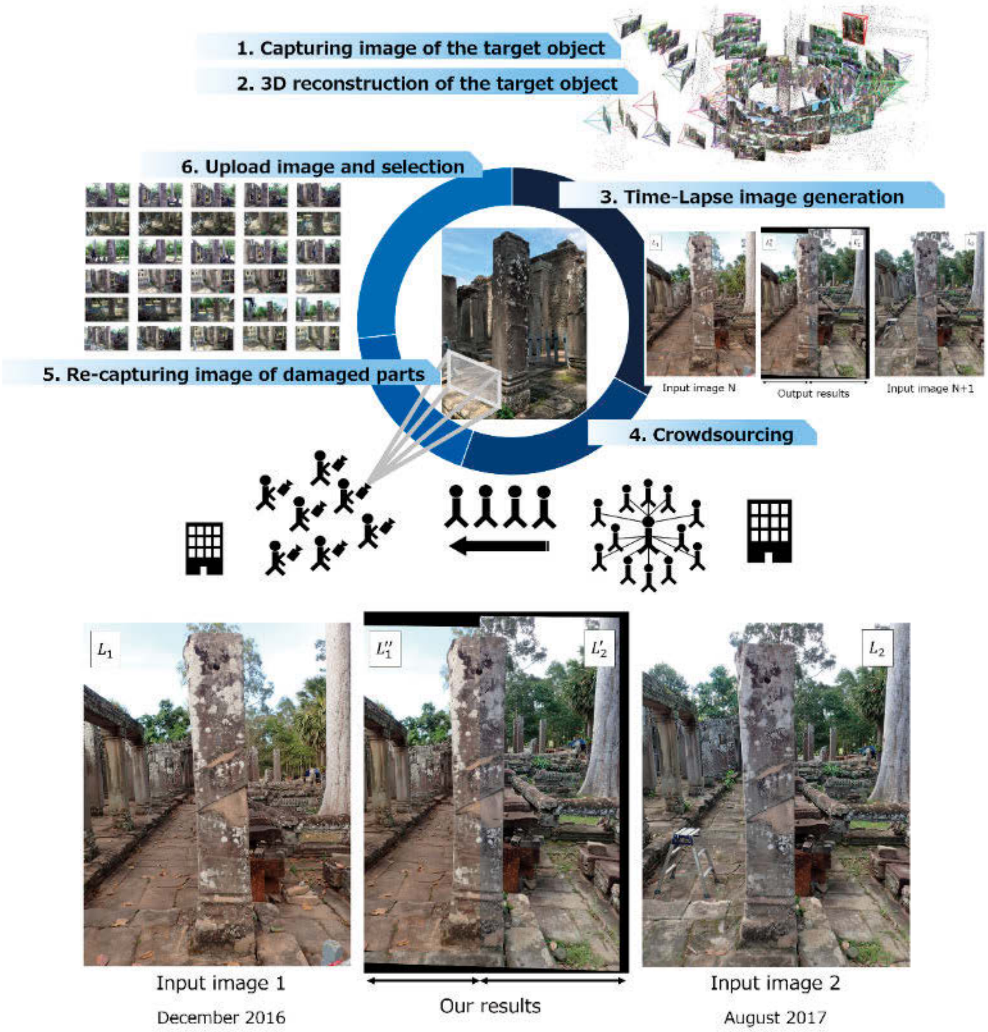

Figure 14. (Upper) Flow of time-lapse image generation using image-based modeling by crowdsourcing : A detailed time lapse image is generated by looping the processing flows. (Lower) Input image 1 (December 2016). Middle: Result of applying the proposed method using input images 1 and 2. Right: Input image 2 (August 2017).

10.3 Collaboration

1) Memorandum of Understanding (MOU) between Center for Computational Sciences at University of Tsukuba (Tsukuba/CCS) and Center for Vision, Speech & Signal Processing at University of Surrey (Surrey/CVSSP) [March 2017]

The objective of this MOU is for the Participants to promote cooperation with a view to contributing to scientific research and technological development in computational sciences.

The Participants expressed their intention to explore future collaboration between Participants in the following areas: a) Computer Vision; b) Pattern Recognition for Image and Video understanding; and c) Computational Media.

The scope of the above activities and cooperation may be changed or extended to other areas by the written consent of the Participants, with any future collaborative research to be undertaken according to an appropriate written agreement therefor.

Forms of proposed cooperation may include:

- Exchange of personnel, including scientists, graduate students, and postdoctoral fellows;
- Joint organization of workshop, seminars, and similar activities; and
- Exchange of information.

Representatives of the Participants intend to meet, as appropriate, to review the progress of their cooperation.

2) Memorandum of Understanding for the Development of Research Collaboration between CURTIN UNIVERSITY and UNIVERSITY OF TSUKUBA [September 2017]

The objectives of the Parties under this agreement are to (a) work together and share information about their organizations to enhance each other's understanding of each Party's scientific capabilities and requirements subject to confidentiality requirements of each Party, and (b) establish a working relationship targeted to the Parties' specific scientific requirements and interests.

The Parties agree to cooperate to (a) organize a committee of representative research scientists and academics from each Party to visit each Party's facilities to investigate the areas of possible collaborative research and development projects; (b) encourage joint research projects which are externally funded, and (c) encourage Exchange between the Parties of staff and students.

The costs incurred by a Party in facilitating the activities associated with this cooperation, including any exchange of staff and postgraduate research students between the respective institutions, will be the sole responsibility of that institution unless other arrangements have been agreed by the Parties in writing.

The Parties will use their best endeavors to foster scientific research collaboration between the institutions throughout the term of this Memorandum of Understanding.

3) Other Collaborations

In addition to the normal academic collaborations, which include faculty members inside University of Tsukuba and researchers in other universities, we have established the collaboration outside the academic organizations too.

[Industrial companies]

Yahoo Japan Corporation, 2501 Inc., Toyota Motor Corporation, NEC Corporation, Hitachi Ltd.

[Organization / goverment]

2017 Visualization of Joint Positions in Badminton Player (with Nippon Badminton Association)
Responsible for joint position estimation by video processing.

2019 Proactive Preservation Activity of World Heritage (with Japanese government team for Safeguarding Angkor)

Responsible for generating time-series change images of cultural heritage buildings.

More extensive collaboration with other universities is also being conducted to promote our research activities.

[Research alliances]

2014-2019 JST CREST, "Social Imaging project" (PI: Prof. Kenji Suzuki, University of Tsukuba) with Keio Univ.

2016-2021 JST CREST, "Cyborg Crowd project" (PI: Prof. Atsuyuki Morishima, University of Tsukuba) with Shizuoka Univ. Kyoto Univ. Toyama Univ.

10.4 Future Plan

We will continue the current research topics and extend the application fields. At the same time, the fundamental computer vision technology and advanced VR/AR/MR should be investigated to promote computational media in our community. A couple of intensive research issues are shown below.

・Multi-View Visual Media (Free-Viewpoint Video)

We aim to install our multi-view media system into actual events held, such as sports events, surgical operations, child education, and video surveillance. Real-time processing of multi-view video shooting, free-view video generation, visual data transmission, and presentation on a mobile terminal will be implemented in a live broadcast. Advanced contents generation will be realized by automatic camera work generation combined with AI, multi-view video browsing method linked to conventional video media such as broadcasting and large monitors, and next-generation teaching device linked to multimodal-media.

・Advanced scene recognition based on 3D shape restoration technology

We aim to develop scene recognition technology using 3D shape information restored from multi-view images. Specifically, we will research on determining the collapse of buildings and heritage sites, estimating the shape and position of human organs, and managing work progress at construction sites and resource mining sites.

・Proactive preservation activity of cultural heritage

Advanced Computer vision support with high accuracy of 3D shape and color estimation in a wider area over a long time period should be established. We aim to support Angkor Thom Bayon Temple, and Sumpu Castle Park currently.

・Human vision behavior analysis in VR

Immersive VR technology can be an important issue to unite the data world and the real world, so it is considered to be a key concept of computational media. Especially, sport application and working situations would be critical as the actual experiences are sometimes precious and challenging to prepare the same situation for training.

・Athlete performance analysis

Among the development of the immersive VR for behavioral analysis, specific athlete action can be measured, and they could be promising evaluation indices in sport sciences. Some are sole pressure, heart rate, player position and speed, and acceleration, etc.

・Mobility support as assistive technology

Our computer vision and sensor technology could be useful for people who need help to move around in cities, streets, buildings, and rooms. By collaborating with researchers in transportation engineering, we also search for the possibility to change the shape of our society.

10.5 Publications

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38. Hidehiko Shishido, Hansung Kim, Itaru Kitahara, "Super Long Interval Time-Lapse Image Generation for Proactive Preservation of Cultural Heritage Using Crowdsourcing," The 3rd IEEE Workshop on Human-in-the-loop Methods and Human Machine Collaboration in BigData (IEEE HMData 2019), pp.4632-4637, 2019.
39. Naoto Nohara, Hidehiko Shishido, Itaru Kitahara, Yoshinari Kameda, "Pitching Form Evaluation Based on Elbow Position by a Monocular Camera", IWAIT2020, 4 pages, 2020.
40. Kohei Yamasaki, Hidehiko Shishido, Itaru Kitahara, Yoshinari Kameda, "Evaluation for Harmonic Location Estimation System of Image Retrieval and SLAM", IWAIT2020, 4pages, 2020.
41. Oto Takeuchi, Hidehiko Shishido, Yoshinari Kameda, and Hansung Kim, "Image-Quality Improvement of Omnidirectional Free-Viewpoint Images by Generative Adversarial Network," 15th International Conference on Computer Vision Theory and Applications, pp.299-306, 2020.

10.6 Grants

[Kaken by Japan Society for the Promotion of Science]

1. "Spatio-Temporal Analysis and Mixed-Reality-Based Visualization of Video Images of Environmental Cameras toward Safe and Efficient Viewing," by Grant-in-Aid for Scientific Research (B), 2011-2014. (ID:23300064) 13,520,000 JPY.
2. "Enhancing Image Quality of the 3D Free-Viewpoint Video in Large-Scale Space Utilizing Player-Billboard Method," by Grant-in-Aid for Scientific Research (B), 2013-2016. (ID:25280056) 16,900,000 JPY.
3. "Communicative instruction media using X-person perspective video," by Grant-in-Aid for Scientific Research (B), 2017-2020, (ID: 17H01772) 17,550,000 JPY.
4. "Establishment of Pedestrian and Personal Mobility Navigation Technology Based on Pre-recorded Route Video Research Project," by Grant-in-Aid for Scientific Research (B), 2017-2020. (ID:17H01773) 16,250,000 JPY.
5. "Visualization of Joint Positions in Sports Player Images Utilizing Artificial Intelligence," by Grant-in-Aid for Young Scientists (B), 2017-2018. (ID:17K13180) 4,030,000 JPY.
6. "Effectiveness Analysis of Sport Skill Acquisition under Pressure Control," by Grant-in-Aid for Challenging Research (Exploratory), 2019-2021. (ID:19K22857) 6,110,000 JPY.
7. "Visualization of Time Series Change in 3D Reconstruction of Cultural Heritage Buildings," by Grant-in-Aid for Young Scientists, 2019-2020. (ID:19K13416) 4,290,000 JPY.

[Other public funds]

1. "Estimation Method of 3D Skeleton Position in Sparsely Arranged Multi-view Camera Images," by CREST AIP Challenge Program, Japan Science and Technology Agency, 2017. 1,000,000 JPY.
2. "Research on Heart Rate Estimation based on Markerless 3D Joint Position Information," by CREST AIP Challenge PRISM Acceleration Support Program, Japan Science and Technology Agency, 2018. 3,900,000 JPY.

[Academic consulting]

1. 2016 Yahoo Japan Corporation, "Research-Development and shooting experiment for realizing free-viewpoint video services," (500,000 JPY).
2. 2016 2501 Inc., "Academic consulting utilizing academic knowledge and practical experience in demonstration experiment of free-viewpoint video capturing and generation system" (550,000 JPY).
3. 2017 2501 Inc., "Academic consulting utilizing academic knowledge and practical experience in demonstration experiment of free-viewpoint video capturing and generation system" (500,000

JPY).

[Cooperative researches with corporations]

1. 2014 Yahoo Japan Corporation ,"Viewpoint movement in ultra-high resolution multi-view images", (400,000 JPY).
2. 2015 Toyota Motor Corporation, "Fundamental research for realizing a highly accessible society", (1,500,000 JPY).
3. 2016 Toyota Motor Corporation, "Fundamental research for realizing a highly accessible society", (1,500,000 JPY).
4. 2017 2501 Inc., "Research-development on advanced video media based on multi-view video processing", (2,500,000 JPY).
5. 2018 NEC Corporation, "Multi-view camera calibration in dynamic environment" (2,000,000 JPY).
6. 2019 NEC Corporation, "Multi-view camera calibration in dynamic environment" (2,000,000 JPY).
7. 2019 Hitachi Ltd., "3D scene recognition for outdoor sites", (3,660,000 JPY).

[Commissioned researches]

1. 2016 Japan Badminton Association, “3D motion analysis of badminton players”, (300,000 JPY).
2. 2018-2019 MEXT Society 5.0 Realization Research Support Project (Osaka-univ), “Multimodal data extraction of sports scene” (7,000,000 JPY).

CCS Report: PART III

Strategy and Future Plans of Center for Computational Sciences

February 2020

Center for Computational Sciences
University of Tsukuba

Table of Contents

1 The Strategy of CCS

1.1 Introduction

This document, CCS report: PART III, describes the strategy and future plans of the Center for Computational Sciences (CCS), University of Tsukuba. The strategy focuses on a time frame of 2020-2025. The report has been prepared for the review of the Center scheduled from February 19th to 21st. The purpose of the review is to receive the evaluation from outside on the research activities and their outcomes of the CCS in the light of the founding objective, and to make recommendations from a viewpoint of future advances. Since the details of research outcomes are presented in a separate report, this report concentrates more on the strategy and future plans of the CCS.

1.2 Mission and Role of CCS

As described in PART-I of this report, we like to define the mission of the CCS again: **The mission of the CCS is to promote scientific researches by means of computational methodology, through the development of leading-edge computing systems and their applications in codesigning concept to advanced sciences by worldwide researchers.**

In the history of 28 years including the first 12 years as the former organization, Center for Computational Physics, we have been continuing the research under the collaboration of various scientific fields including particle physics, astrophysics, nuclear physics, quantum condensed matter physics, life science, and environmental science, with the computer science fields including high performance computing technology and informatics. This is a unique organization to provide a cross-field research opportunity among all of these scientific regions under not just the policy of University of Tsukuba but also Ministry of Education, Sports, Culture, Science and Technology (MEXT) toward the interdisciplinary research lead by state-of-the-art high speed computing technology. Actually, the CCS is recognized as the highest level of research organization in Japan to lead the codesigning and HPC technology contributing cutting edge of computational sciences in Japan. Moreover, the CCS is also recognized as one of the top level research centers for HPC and computational sciences in the world. Our activities have been evaluated through a large number of publications over varying research fields. Another presence of our activities has been displayed at the research exhibition at SC (Supercomputing) Conference

In USA and ISC (International Supercomputing Conference) in Germany. Especially, the CCS is the first Japanese university to start our own exhibition booth at SC on 1997.

The uniqueness of the CCS is well known in Japan as the first codesign center under collaboration among computational domain science and computer science fields. Currently, we have 43 faculty members and about 2/3 of them belong to the computational domain science fields while other 1/3 are in computer science field. It is well balanced organization for codesigning and ideal collaboration for interdisciplinary research. In Japan, nine national universities have their own supercomputer centers, however the CCS is only one which was established as a research center while all others were established as service centers to operate supercomputers for nationwide utilization by researchers. Without this research formation, it is impossible to build a true codesign center in Japan.

As described above, the CCS is recognized as the leading center both for supercomputing and computational domain sciences in Japan. It means that our mission is not just the research in our university, but also to be the leader in these research regions in Japan and even the world. For this purpose, we have been developing our original codes for computational sciences in various fields. They are mainly supported by governmental budget as well as education of young researchers who can develop their own application codes. Usually these codes are developed by the domain scientists, however in our center, the research team in computer science field supports the development, enhancement or porting to advanced systems such as accelerated supercomputer with GPU or FPGA. All these activities are just available under our unique organization of the CCS.

For the supercomputer development, we have been also introducing our original systems based on tight discussion with application researchers toward high sustained performance without just chasing the new technology and peak performance. CP-PACS built in 1996 was our monumental achievement where the only one system from Japan lead by a university project supported by government to build the world fastest supercomputer. Through the processor and system design, we surveyed the characteristics of target applications (mainly on particle physics) and discussed with the system vendor (Hitachi Co., Ltd.) to introduce unique feature of Pseudo Vector Processing with Sliding Window, which is a patent awarded technology to introduce the pseudo vector calculation scheme on scalar processor. All the following systems could not have a chance to develop the CPU from scratch, we continued to develop systems with gravity accelerators for astrophysics (FIRST), high bandwidth memory and network (PACS-CS), introducing FPGA to support GPU communication (HA-PACS), and new many-core technology (COMA and Oakforest-PACS). The latest our challenge is to combine the GPU and FPGA computing in a single system toward highly efficient accelerated computing (Cygnus). It is also impossible in the ordinary supercomputer centers in other universities in Japan.

Through the long history of such activities, we have been contributing to the development of national projects to develop flagship supercomputers and their applications. Before K Computer project started, MEXT was interested in our new concept of low-power and high-performance accelerated computing. Our plan was not accepted, but core researchers in application and system fields of the CCS were invited to the design working group of K Computer to contribute to the processor and system design of it. Also, HPCI Projects for application development in various research fields started, and the CCS was selected as the core organization of Field-5, fundamental science to lead the application development on particle physics and astrophysics. The follow up project after K Computer named "Post-K" Computer development, again the CCS proposed an extremely high degree of SIMD accelerator toward Exascale computing in the feasibility study phase. The proposal was not accepted finally due to lack of partner vendor within a reasonable budget, however the core researchers were invited to the design team of Post-K Computer again. They contributed to the detailed design and pre-evaluation of performance of the processor and network. Also, the CCS was selected as the core organization for Post-K phase of HPCI Projects (Field-9 of fundamental science).

In conclusion, we have the following missions and roles to lead the computational science research:

- Leading the cutting edge computational sciences in various fields under the collaboration among domain scientists and computer scientists
- Developing advanced supercomputers under codesigning concept by the collaboration of application and system researchers
- Providing advanced supercomputers to be shared by nationwide computational science projects
- Contributing to national projects on system and application development such as K Computer or Fugaku Computer

1.3 Multidisciplinary Computational Sciences

The core concept of our CCS research is named Multidisciplinary Computational Sciences, which means the advanced science of today should be established not just on a single and narrow field of research but wide variety of coverage over multiple research fields such as combination of physics and chemistry, physics and computer science, astrophysics and bioscience, and so on. As described above, ordinary codesigning is a sort of bridging over application field and computer science. However, what we aim as Multidisciplinary Computationl Sciences covers even the cross fielding over multiple domain sciences. One of the instances is our Department of Computational Medical Science. The collaboration between science and engineering is not new anymore, however we focus here the collaboration among science, engineering and medicine. There is borderless possibility of cross-research such as computational astrobiology, big data analysis on human's sleeping activities, optical bioimaging commonly used for astrophysics radiation transfer and human body scan, 3D CG technology for surgery operation, etc. This is our advantage to cover such borderless collaboration mostly in our center, but here we need another factor of medicine. Fortunately, Department of Medicine in University of Tsukuba is the top level organization and we can have a tight inter-organization relationship with them. Since the CCS is ranked as R1 Center in the university which aims to establish the world top class research and a special support from University of Tsukuba, it is possible to make such a collaboration with another top level organization.

We have been leading this concept of Multidisciplinary Computational Sciences under the program of our supercomputer resource sharing named "Multidisciplinary Collaborative Research Program" (MCRP) for long time. It is basically a large amount of resource sharing on our supercomputer resources, but we also promote to organize a multidisciplinary collaboration team among different fields. Especially for an advanced technology such as FPGA, corresponding researchers in the CCS join the project to support their development and implementation on Cygnus supercomputer. It is our unique activity which is not possible in other supercomputer centers in Japanese universities.

We consider the future of computational sciences diverse in wide variety of fields and we believe that our concept of Multidisciplinary Computational Sciences create the new horizon of computational science research.

2 Future Plans of CCS

2.1 Supercomputer Development

We will continue our way of codesigning based on advanced computing technologies and scientific computing scheme toward the next generation supercomputers. Of course, there is a limit on budget and manpower so that we cannot achieve the level of national flagship machine. However, it is possible to show what is the key technologies in the next generation where various physical limits are supposed such as the minimum semiconductor design rule, power consumption, footprint, bandwidth of memory and interconnect, memory capacity, etc. This is why many people are interested into the accelerated computing and actually the world top level supercomputers are mainly equipped with accelerators such as GPU.

Here, we consider that the GPU is not omnipotent and the coverage of applications will be limit in the near future because the system performance enhancement by enlarging the system will reach to the end. For instance, we cannot enlarge the system keeping the same amount of memory per core. In the past 30 years, system size of supercomputers has been increased in the number of nodes, CPU cores, memory capacity, etc. They are improved as the aggregated performance or counts of each component. However, when these factors are reaching their limits, "capacity enlargement" is no more the solution. In the next generation, the latency is much more important than throughput. It means that the strong scaling is the way to improve the performance.

2.1.1 PACS-X and PACS-XI

Cygnus is a proof of concept system to display what the concept of AiS can make progress in the next generation's accelerated computing. We started this project as PACS-X Project with multi-hybrid accelerators. Actually the Cygnus system was designed and implemented, however we think the system size is not enough to show its true performance as in the strong scaling.

The limit of GPU is that it is SIMD-based throughput system. Each core of GPU has relatively low performance but a collection of large count of cores leads to extremely high performance. To save the power consumption, high degree of SIMD controlling is introduced, thus the application field is limited. We will apply larger amount of budget to build a really scalable system to show our concept is correct both for strong scaling and weak scaling by its architecture. We are planning to apply another phase of system development to complete the Cygnus system as true PACS-X

System.

Fig. 1 shows the future plan of all supercomputer centers at national universities, which is published from MEXT based on each university's future plan. These university machines are recognized as in Tier-2 category while K Computer and Fugaku are in Tier-1 category. Most of bars in the future are just plans, but each university conceptually considers their own system deployment policy. Here, we declared the next developed system in the CCS is named PACS-XI (no nickname yet) with advanced technology with up to 100PFLOPS performance. "TPF" stands for Tehnology Path Finder in Japan's HPCI system development concept. In the CCS, we have been developing TPF style of machines under codesign among the application and system. The detailed plan is under construction, but we expand our concept of multi-hybrid accelerated computing in the next step.

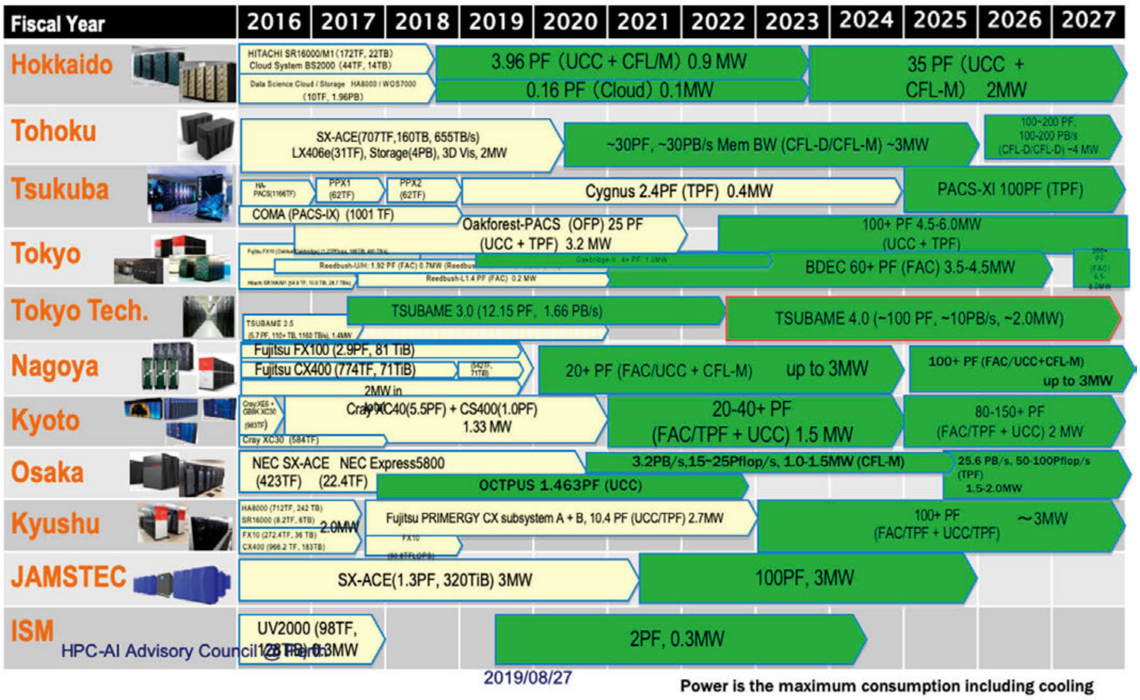

Fig. 1 Supercomputer deployment plan of all national universities in Japan

2.1.2 Post-OFP Project in JCAHPC

When we launched Joint Center for Advanced HPC in Japan (JCAHPC), one of the clear objectives was to install the fastest supercomputer in Japan because we believed that the many-core architecture was the most promised way of general purpose processor for high performance under certain power consumption. Actually, we merged our budget for supercomputer procurement and finally built the Oakforest-PACS (OFP) System with 25 PFLOPS os peak performance as well as 13.4 PFLOPS os HPL performance, ranked at #6 in TOP500 List on

November 2016. Even after a new GPU cluster named ABCI in MITI, the OFP is still the largest Tier-2 system in HPCI resource sharing.

The OFP System is planned to complete its working life on March 2022 which is the end of FY2021. We have a plan to continue the activity of JCAHPC after the end of OFP and providing the top-level resource in Tier-2 category. Currently, the system is just called Post-OFP. Again in Fig. 1, University of Tsukuba and the University of Tokyo will share a new machine without name to achieve more than 100PFLOPS with the cluster technology with some advanced one. Here, the Post-OFP System will be based on a general purpose CPU with many-core architecture for the continuation after the OFP for a large number of nationwide researchers under HPCI and MCRP program (MCRP is only in our university). We started several discussions with vendors, and the procurement will be started in this year. As shown in Fig. 1, we will complete the system installation within FY2022.

2.2 Activities as the world top level center

As R1 class center in University of Tsukuba, our mission is to proceed the world top level research as a distinguished codesign center. For this purpose, we are still on our way, however all the research activities reported in this report PART-I and PART-II aim to this goal. One of the issues we focus on now is the international collaboration. As reported in PART-I, we have been collaborating with other top-level research centers in USA, UK and Korea. We are expanding the research MOU for widely spread research topics which are covered in the research divisions at the CCS.

The reason why we focus on the MOUs is that we strongly believe the MOU-base tight collaboration leads to a great success in the specific topic and finally to create an excellent research result. Here, the internationalization of the center is also important because MEXT started to award the top-level centers as International Distinguished Research Center. The real collaboration with world top-level institute and the volume of coauthored publications strongly impact for the evaluation. Of course, it is not our real purpose to be recognized as such a center, but the true goal is establishing the strongest codesign center for international multidisciplinary computational sciences.

Toward this goal, we negotiate with the university for better research environment, stronger research team with high quality of researchers, research budget and other support. The university is respecting to our activities but also the request and KPI to be cleared are at the hardest level in the university. We will continue our effort toward the goal.