Research Activity Update of CCS

Taisuke Boku
Director, Center for Computational Sciences
Unviersity of Tsukuba


Organization of CCS

Taisuke Boku

Kazuhiro Yabana

- Director
  - Steering Council
  - Strategic Planning Headquarters
  - Administrative Council
  - Personnel Committee
  - Researcher Meeting
- Deputy Director
- Research Project Offices
  - Project Office for Exascale Computational Sciences
  - Project Office for Exascale Computing System Development
  - Project Office for HPCI Strategic Program
  - Project Office for AI & Big Data
  - Project Office for HPC System Development and Management
  - Promotion Office for Computational Sciences
- Director for Organization Strategy
  - Liaison Office for Multidiscplinary Computational Sciences
  - Bureau of Public Relationships and Strategy
- Director for Cooperative Research
  - Board of Cooperative Research
  - Administrative Committee for Cooperative Research
- Administrative Committee for Computer Systems
- Joint Center of Advanced HPC
- Department of Computational Medical Science
- Research Divisions
  - Particle Physics
  - Astrophysics
  - Nuclear Physics
  - Quantum Condensed Matter Physics
  - Life Science
  - Global Environmental Science
  - High Performance Computer Systems
  - Computational Informatics

Faculty 45
Professor 17
Associate Prof. 10
Lecturer 2
Assistant Prof. 11
Assistant Prof. 3 (TT)
Assistant Prof. 2 (International-TT)

as of Sep. 2022

Research Divisions and Leaders

- Computational Science
  - Particle Physics (Y. Kuramashi)
  - Astrophysics (K. Ohsuga)
  - Nuclear Physics (T. Nakatsukasa)
  - Quantum Condensed Matter Physics (M. Otani)
  - Life Science
    - Biological Function and Information (Y. Shigeta)
    - Molecular Evolution (Y. Inagaki)
  - Global Environmental Science (H. Kusaka)
- Computer Science
  - High Performance Computing Systems (T. Boku)
  - Computational Informatics
    - Database (T. Amagasa)
    - Computational Media (Y. Kameda)


Y. Kuramashi


K. Ohsuga


T. Nakatsukasa


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H. Kusaka


T. Boku


T. Amagasa


Y. Kameda

Codesigning between Computational and Computer Science

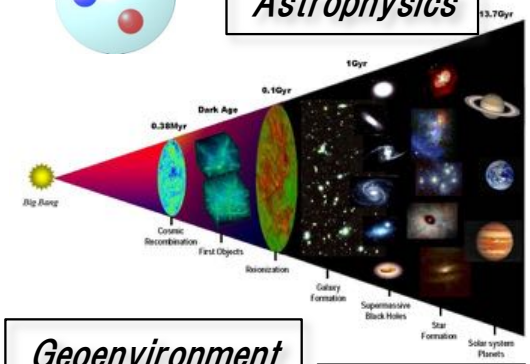
Project Office for Exascale Computational Sciences

Project Office for Exascale Computing System Development

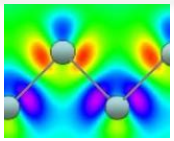
Particle Physics

Nuclear Physics

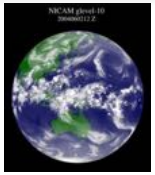
Astrophysics



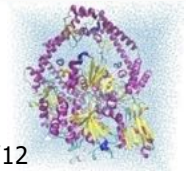
Materials Science



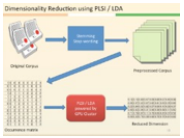
Geoenvironment



Bioscience



Database



Cygnus

Pegasus

➡ Decomissioned

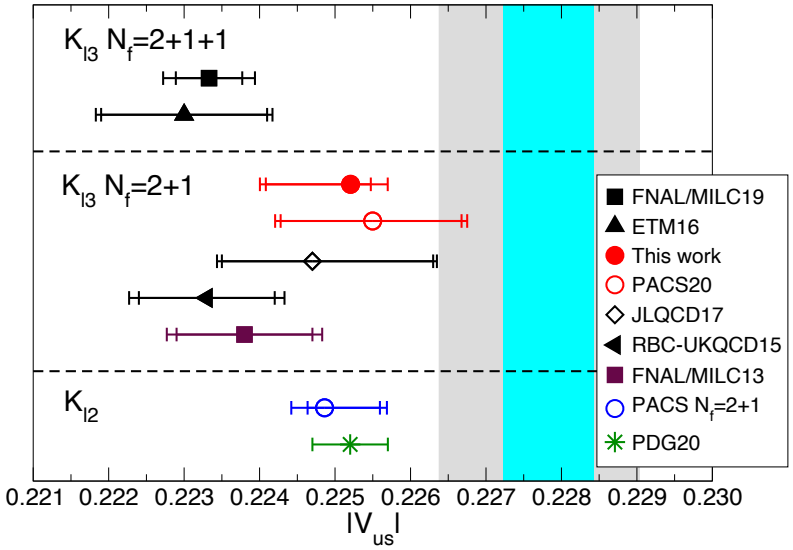
Division of Particle Physics

Topics: Lattice QCD (Quantum Chromodynamics), Tensor renormalization group,
Physics beyond the standard model, QCD at finite temperature and finite density

Lattice QCD simulation

- Large scale parallel computation
- Search for new physics

PRD106(2022)109

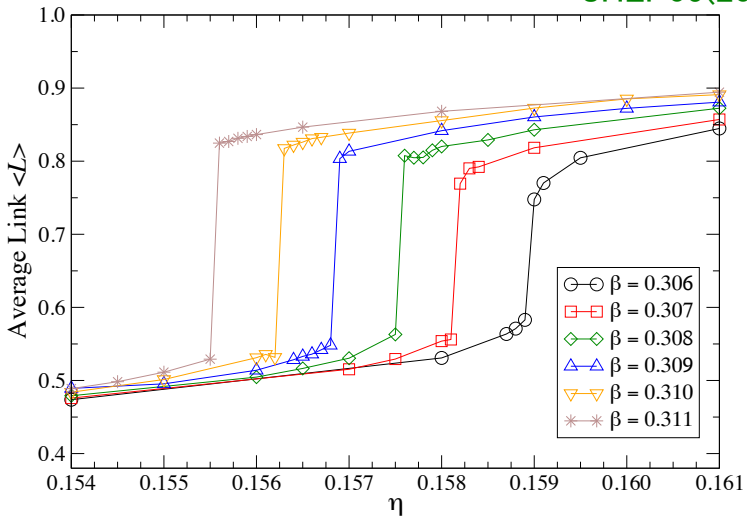


Difference btw the CKM unitarity (cyan) and simulation results (symbols w/ errors)
⇒ hint of new physics

Tensor renormalization group

- Deterministic algorithm
- Free from the sign problem
- Application to finite density QCD, Hubbard model etc.

JHEP05(2022)102



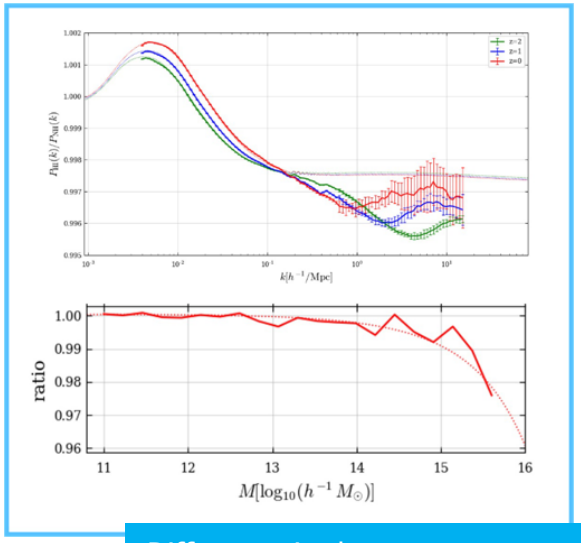
First-order phase transition in (3+1)-dimensional Z_2 gauge-Higgs model at μ =1

Division of Astrophysics

Topics: The birth and evolution of the first stars and galaxies in the universe, the formation and evolution of galaxies and large-scale structures, the formation and evolution of black holes, the formation of planets, and the origin of life in the universe.

Large-scale structure:

Vlasov and Boltzmann simulation of massive neutrinos and self-interacting dark matter

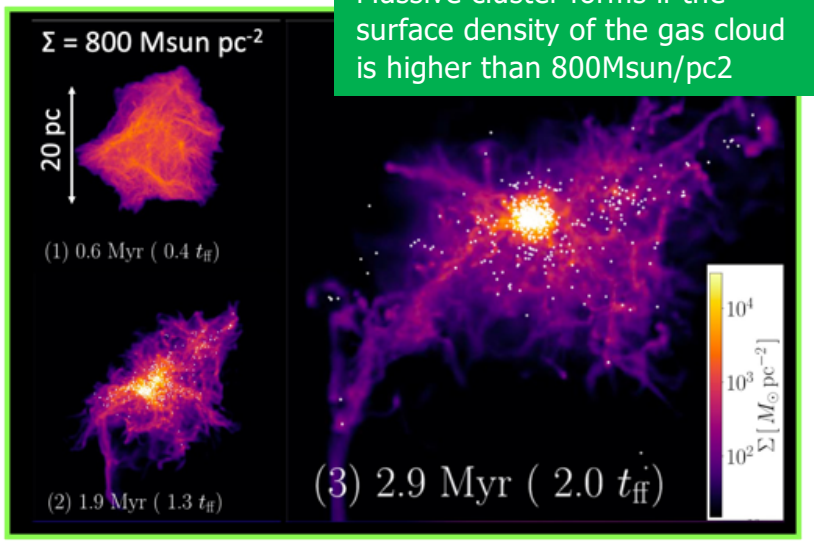


Difference in the power spectra is on the order of 0.5 %.

Star cluster:

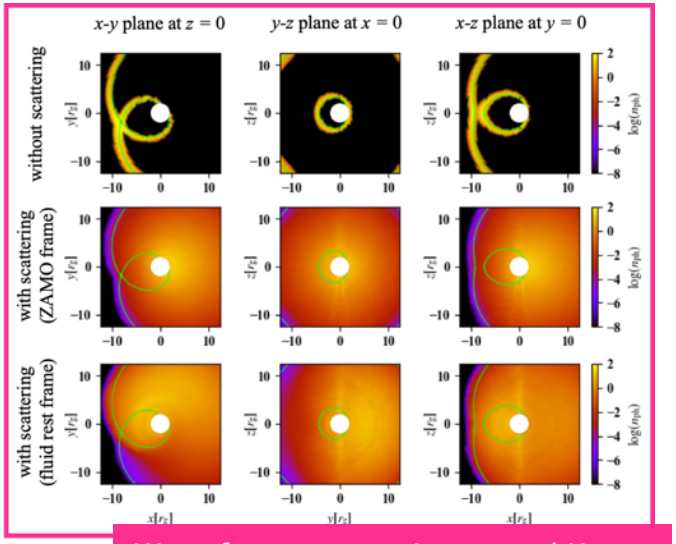
Radiation hydrodynamics simulations of star cluster formation

Massive cluster forms if the surface density of the gas cloud is higher than 800Msun/pc2



Black hole physics:

Development of novel general relativistic radiation transfer code

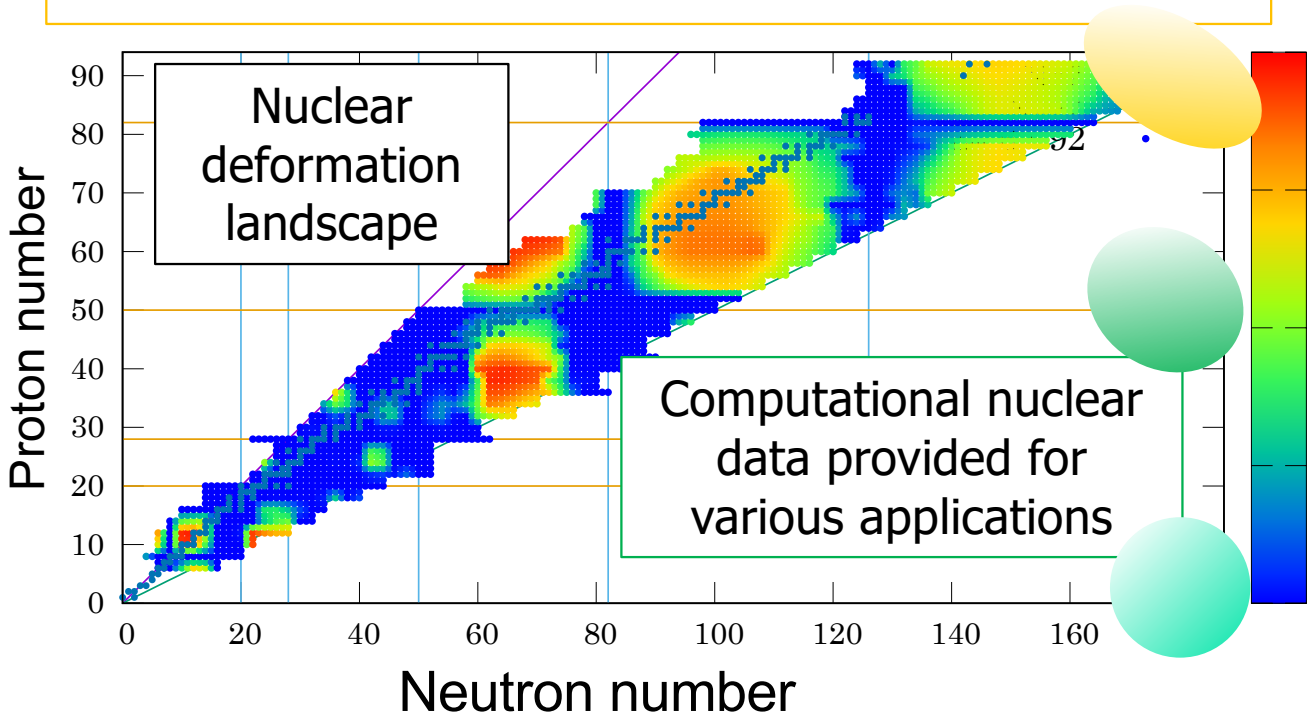


Wave front propagation around Kerr black hole is nicely reproduced.

Division of Nuclear Physics

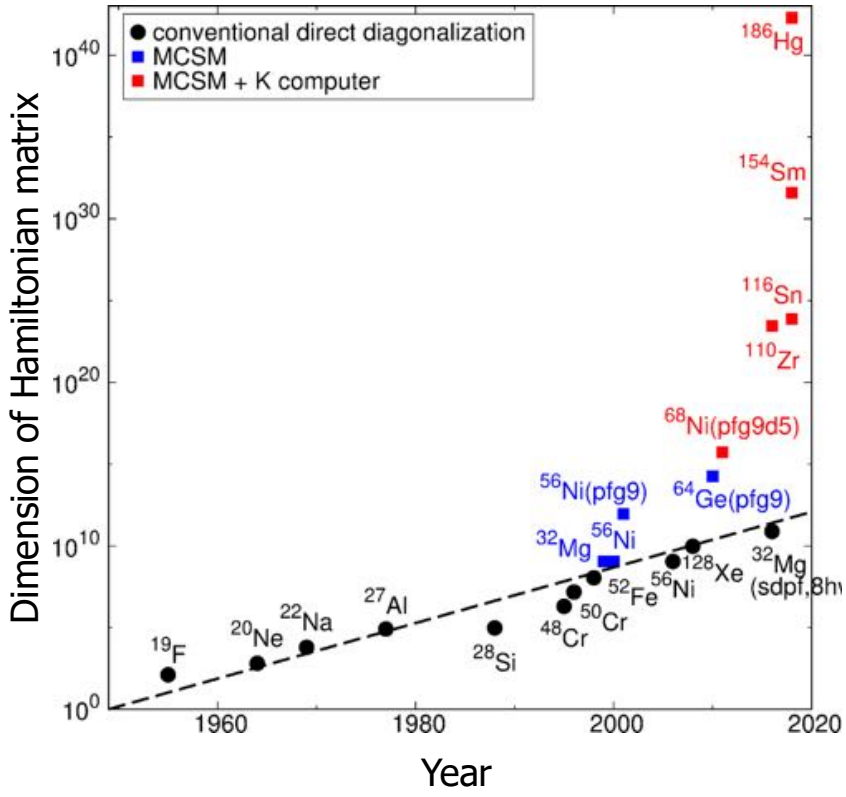
Main research topics

- **Nuclear structure and reaction (fusion, fission, etc.)**
- **Neutron stars and element synthesis in universe**
- **Computational nuclear data**



"KSHELL" code for nuclear shell-mode

This page is for "KSHELL", nuclear shell-model calculation code.



Division of Quantum Condensed Matter Physics

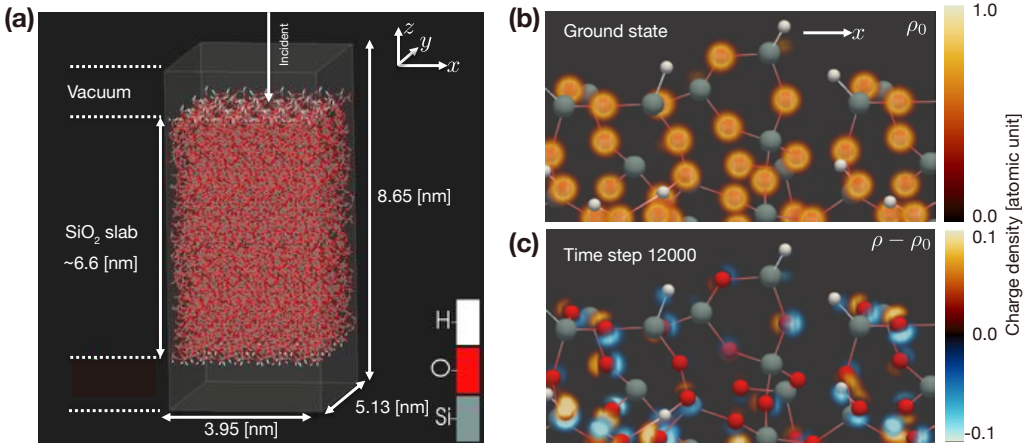
Topics: First-principles computational methods and software developments, nano-optics, ultrafast phenomena, electrochemistry, strongly correlated systems

Developing open-source software SALMON

- Electronic dynamics calculations in first-principles level
- Nano-optics is the main target field

Using SALMON on Fugaku supercomputer

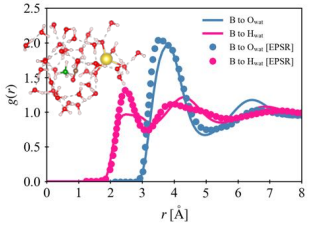
- Electronic dynamics in laser-irradiated glass (SiO_2)
- 10,224 atoms (26,640 electron orbitals) using 27,648 nodes



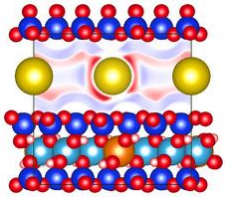
Developing a reliable method for electrochemical reactions: ESM-RISM

- A hybrid simulation method combining first-principles method and classical liquid theory
- Electrochemical-reaction processes is the main target.

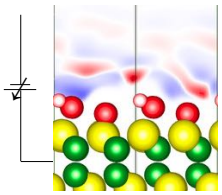
Bulk solution



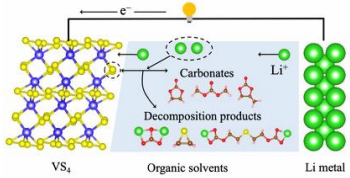
Water containing system



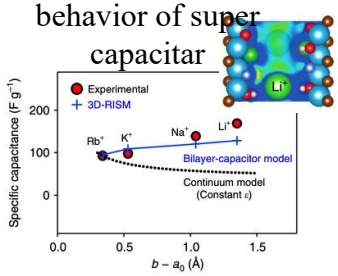
Electrochemical interface



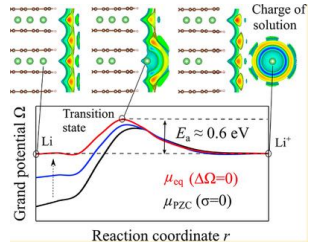
Key reactions in degradation of next generation battery



Cation dependent behavior of super capacitar

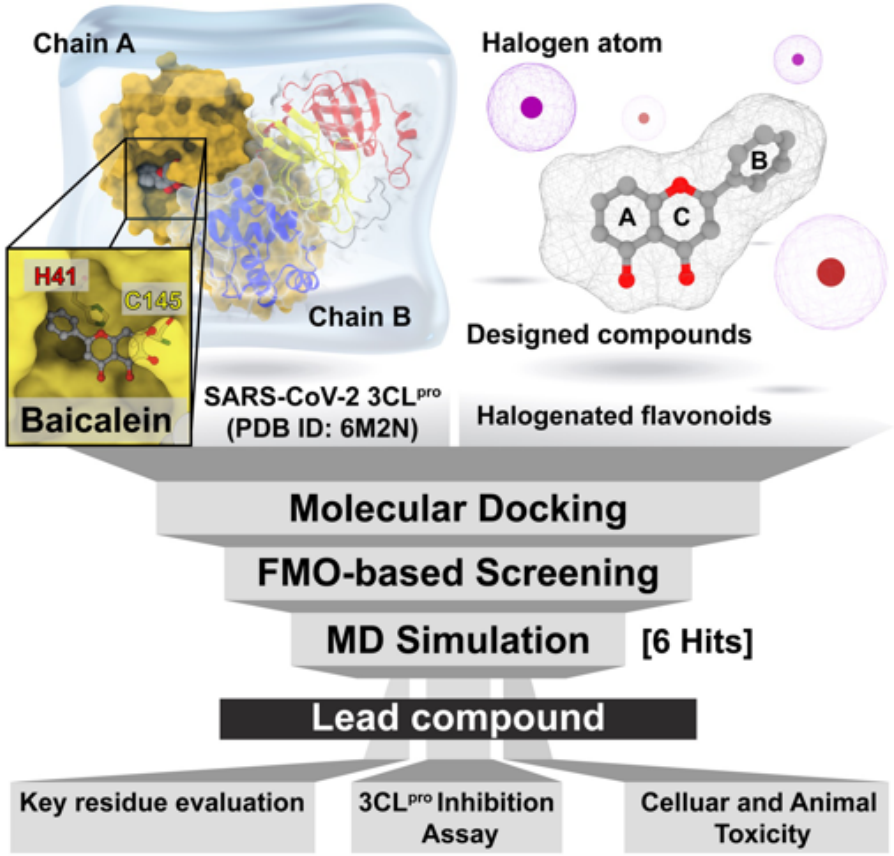


Electrochemical reaction processes @ constant bias



Division of Life science: Biological Function and Information Group

Topics: Molecular dynamics simulation, Quantum chemical calculation, Virtual screening

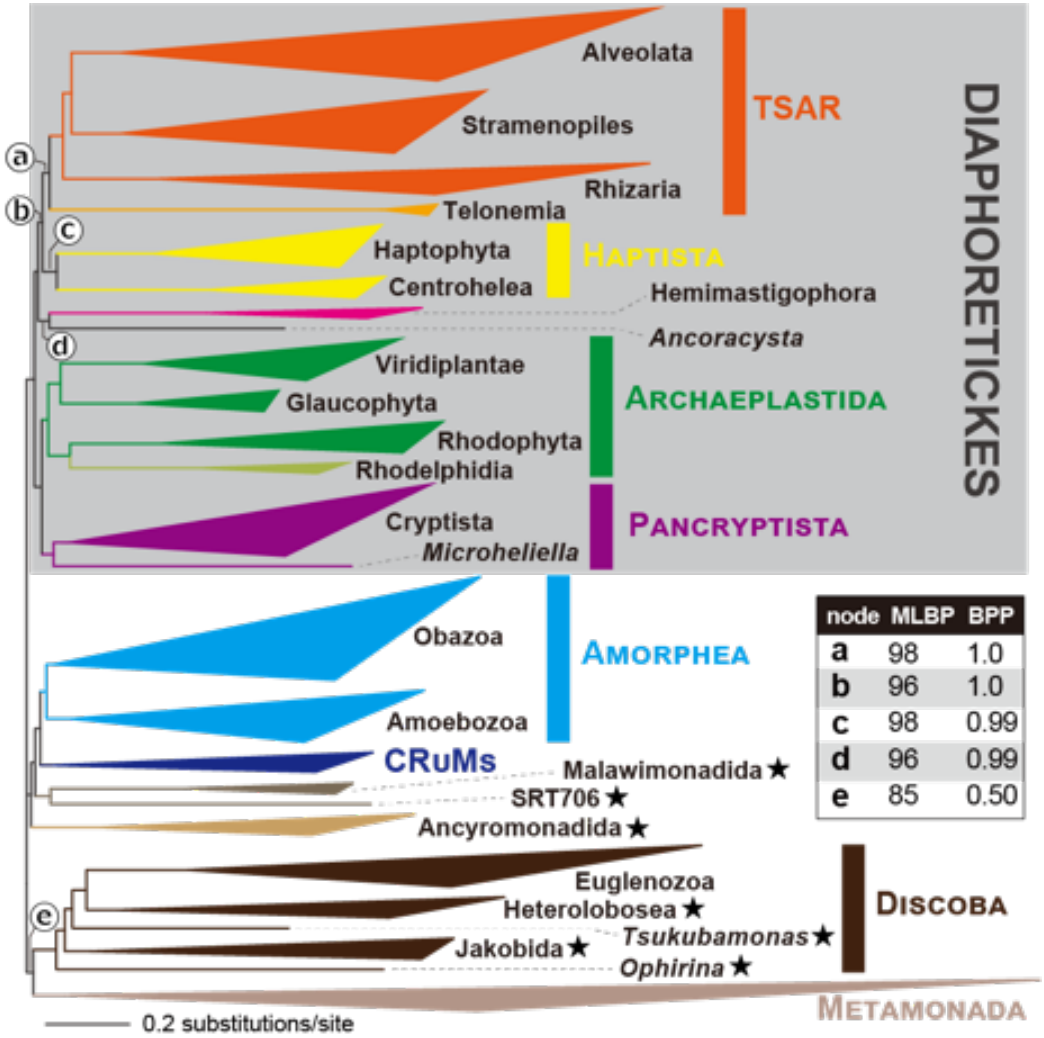


FMO-based virtual screening for Covid-19 M^{pro} inhibitor

We have proposed fragment molecular orbital (FMO)-based virtual screening to predict the molecular binding energy of SARS-CoV-2 main protease (M^{pro}) inhibitors. The integration of quantum mechanical approaches and MD trajectory analysis was used to identify potential inhibitors. We identified a brominated baicalein as a potent inhibitor of the M^{pro} and confirmed its inhibitory activity in an *in vitro* assay. Also, cell toxicity was tested to confirm the applicability.

K. Hengphasatporn, *et al.*, "Halogenated baicalein as a promising antiviral agent toward SARS-CoV-2 main protease", *J. Chem. Inf. Model.* **62**(6), 1498–1509 (2022) (2022).

K. Hengphasatporn *et al.*, "Promising SARS-CoV-2 main protease inhibitor ligand-binding modes evaluated using LB-PaCS-MD/FMO", *Sci. Rep.* **12**, 17984 (16 pages) (2022).



node	MLBP	BPP
a	98	1.0
b	96	1.0
c	98	0.99
d	96	0.99
e	85	0.50

The upper figure is an example of the tree of eukaryotes inferred from an alignment comprising 340 proteins

Division of Life Sciences, Molecular Evolution Group

Our primary interest

We aim to resolve the evolutionary relationship among major groups of eukaryotes.

keywords

Tree of eukaryotes, Genomics, Transcriptomics, Biogeography, Phylogenetic analyses, Phylogenetic artifacts, Organellogenesis, Endosymbiosis.

Recent papers

- Yazaki et al. The closest lineage of Archaeplastida is revealed by phylogenomics analyses that include *Microheliella maris*. ***Open Biol*** 202212:210376
- Yazaki et al. Barthelonids represent a deep-branching metamonad clade with mitochondrion-related oragnelles predicted to generate no ATP. ***Proc Roy Soc B*** 2020 287:20201538.
- Sarai et al. Dinoflagellate with relic endosymbiont nuclei as models for elucidating organellogenesis. ***Proc Nat Acad Sci USA*** 2020 117:5364-5375.
- Nakayama et al. Single-cell genomics unveiled a cryptic cyanobacterial lineage with a worldwide distribution hidden by a dinoflagellate host. ***Proc Nat Acad Sci USA*** 2019 116:15973-15978.

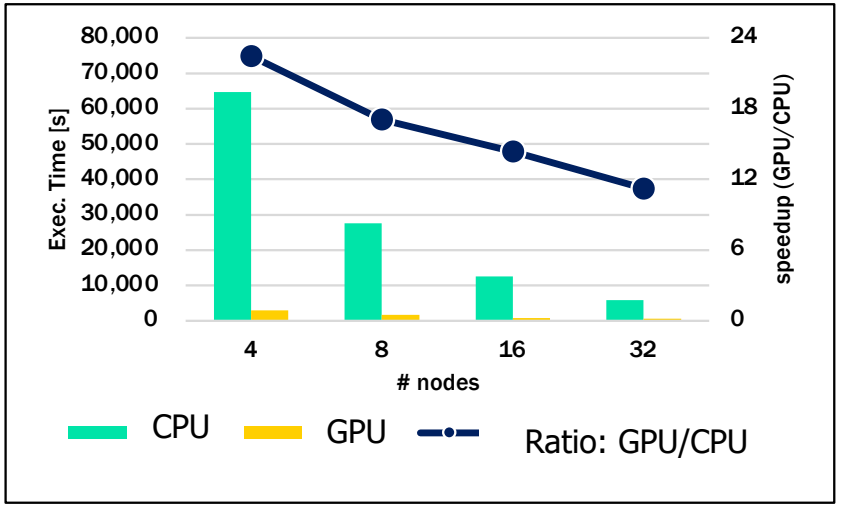
Division of Global Environmental Science

Topics

- Meso- and Micro-scale Urban Climate
- Global-scale General Circulation

Development of city-scale LES model for urban climate studies

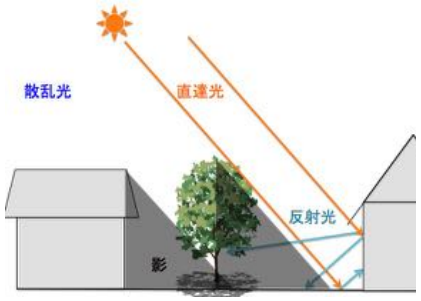
- ✓ Building-resolving LES, Spatial resolution is O(1) ~ O(10) m
- ✓ 3D non-hydrostatic, Bousinessq approximation equations
- ✓ Short- and long-wave radiation models
- ✓ Cloud microphysics model
- ✓ Isolated street tree model
- ✓ 3D multiple reflections of radiations in the urban canopy layer
- ✓ CPU version (MPI+OPM 3D parallelization) and GPU version

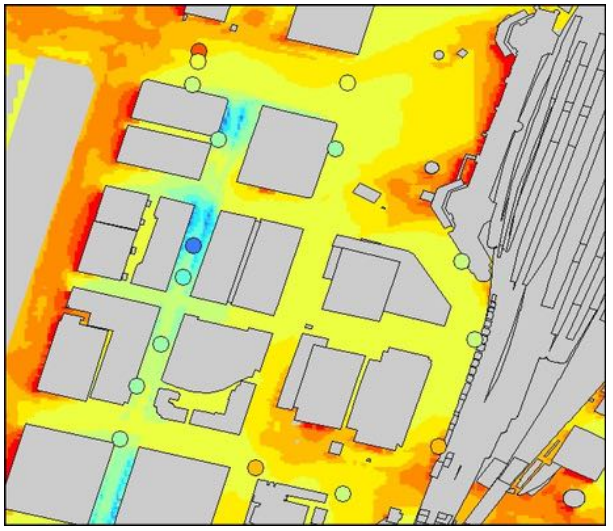


$$\frac{\partial \overline{u_i}}{\partial x_i} = 0$$

$$\frac{\partial \overline{u_i}}{\partial t} + \frac{\partial \overline{u_i}\,\overline{u_j}}{\partial x_j} = -c_p \Theta_0 \frac{\partial \overline{\pi'}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(-\tau_{ij} + 2\nu \overline{S_{ij}}\right) + \frac{g}{\Theta_0}\overline{\theta'}\delta_{i3} + F_i$$

$$\frac{\partial \overline{\theta}}{\partial t} + \frac{\partial \overline{u_j}\,\overline{\theta}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(-\tau_{\theta j} + \kappa \frac{\partial \overline{\theta}}{\partial x_j}\right) + Q$$





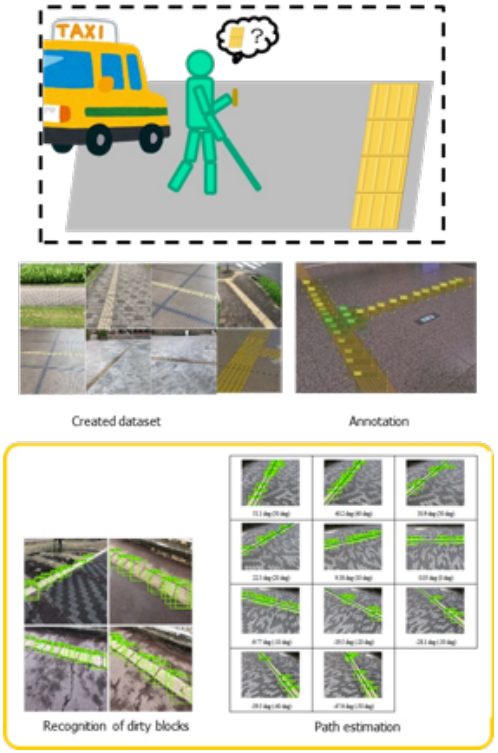
Maximum Temperature around Tokyo Station

Solid circles and background shading indicate observations and simulations, respectively.

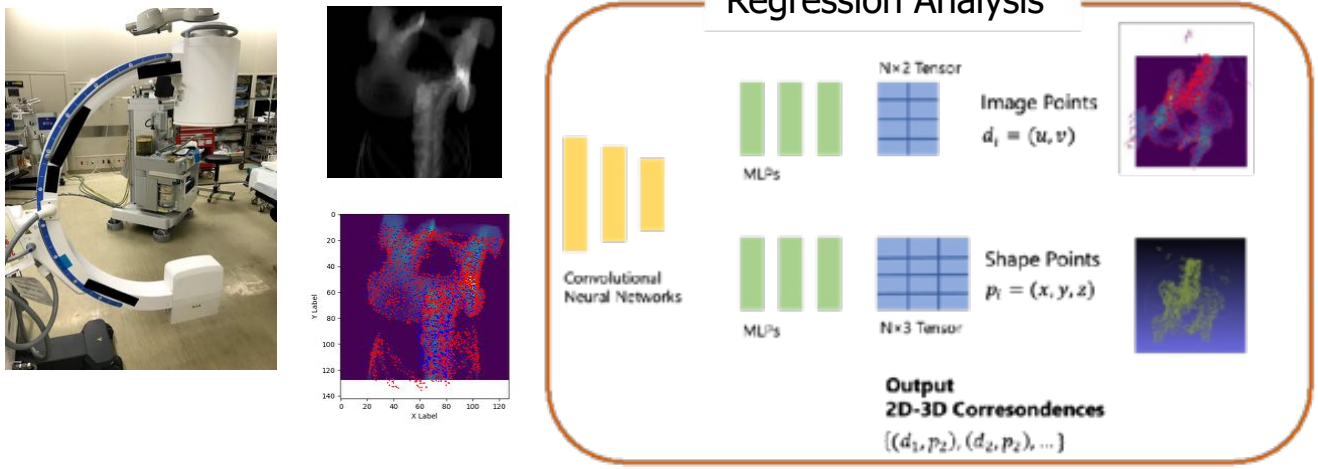
Division of Computational Informatics: Computational Media Group

Topics: Free viewpoint 3D data browsing, 3D shape recovery, computer vision and pattern recognition, sports analysis, assistive technology, industrial applications, 3D surgical vision

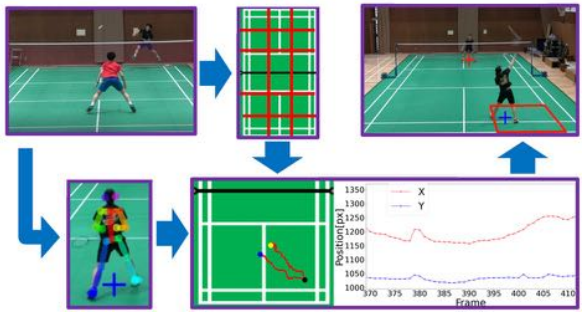
Recognition of Braille blocks by mobile devices and Guidance to the nearest Braille block



Markerless Alignment Method of CT Data and X-ray Fluoroscopic Images Using 3D Reconstruction Deep Network



Shot Detection Method Using Footwork Trajectory in Badminton Video

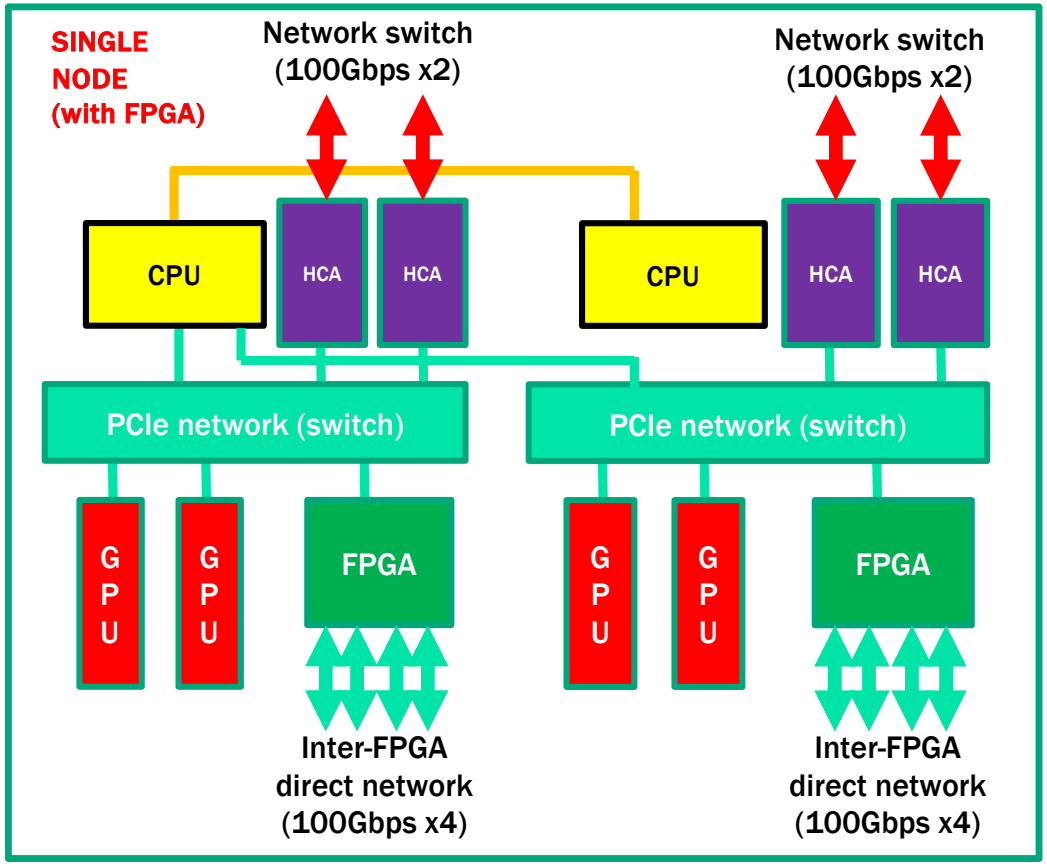


Cygnus System

Computation node	CPU / node	Intel Xeon Gold (SKL) x2 sockets
	GPU / node	NVIDIA V100 x4 (PCIe)
	FPGA / node	Intel Stratix10 x2 (each with 100Gbps x4 links/FPGA and x8 links/node)
	Memory	192 GiB DDR4-2666/node = 256GB/s, 32GiB x 4 for GPU/node = 3.6TB/s
Number of nodes		81 (32 Albireo (GPU+FPGA) nodes, 49 Deneb (GPU-only) nodes) + 4 PMEM Nodes
Interconnection network		Mellanox InfiniBand HDR100 x4 (two cables of HDR200 / node) 4 TB/s aggregated bandwidth
Peak performance		2.56 PFLOPS DP (GPU: 2.2 PFLOPS, CPU: 0.2 PFLOPS, FPGA: 0.6 PFLOPS SP)
Global file system		Lustre, RAID6, 2.5 PB
Programming language		CPU: C, C++, Fortran, OpenMP, GPU: OpenACC, CUDA FPGA: OpenCL, Verilog HDL

Single node configuration (Albireo) of Cygnus

- All nodes in Cygnus are equipped with both IB EDR and FPGA-direct network
- Some nodes (Albireo) are equipped with both FPGAs and GPUs, and other nodes (Deneb) are with GPUs only
- GPU: NVIDIA V100 x4
  FPGA: Intel Stratix10 x2



First target application of GPU+FPGA acceleration ⇨ ARGOT code

Astrophysical Simulation for first objects in the Universe

Two computation elements in ARGOT code: ARGOT method and ART method

- ARGOT method: Point Source processing
- ART method (Authentic Radiation Transfer): Diffused Photon processing

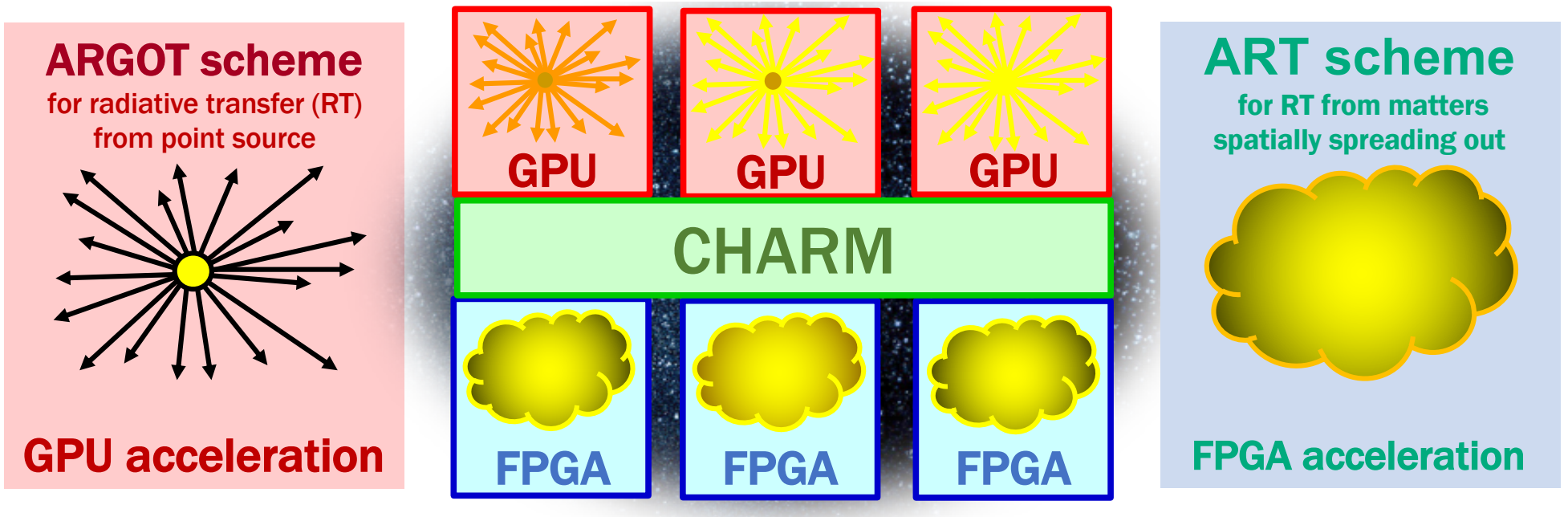
First target application of GPU+FPGA acceleration ⇨ ARGOT code

Astrophysical Simulation for first objects in the Universe

Two computation elements in ARGOT code: ARGOT method and ART method

- ARGOT method: Point Source processing
- ART method (Authentic Radiation Transfer): Diffused Photon processing

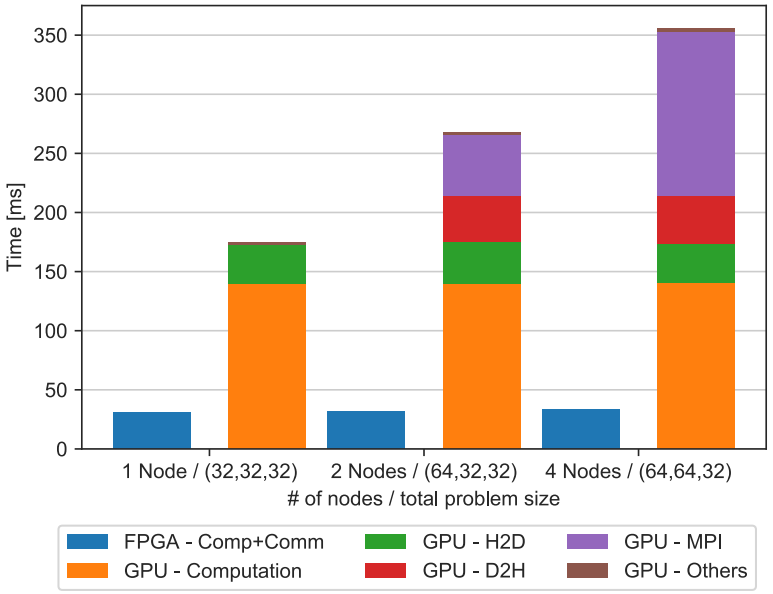
ARGOT (Accelerated Radiative transfer on Grids using Oct-Tree) **code**



CHARM: Cooperative Heterogeneous Acceleration by Reconfigurable Multi-devices

GPU+FPGA=CHARM (Cooperative Heterogeneous Acceleration with Reconfigurable Multi-devices)

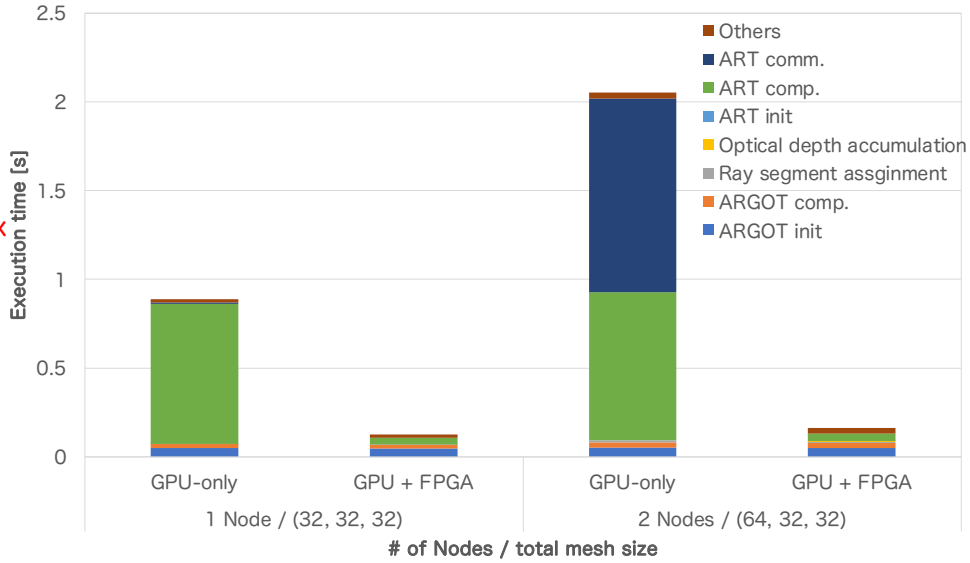
- ART only: weak scaling, GPU vs FPGA



- 1 node
  - GPU+FPGA achieves 6.8x faster than GPU-only
- 2 nodes
  - GPU+FPGA achieves 12.8x faster than GPU-only

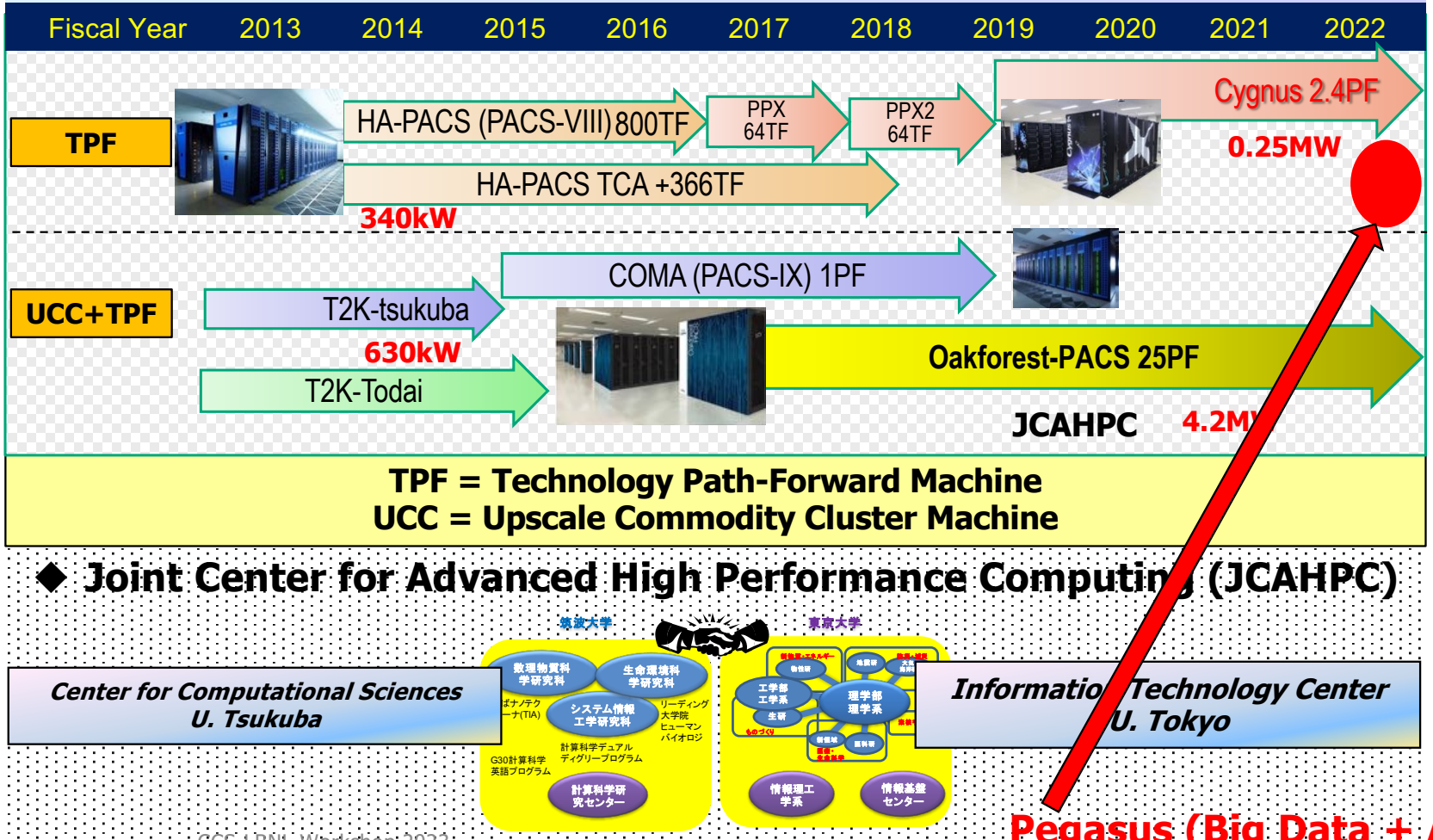
  → combining computation and communication in pipeline

- Weak scaling with 2 nodes (2 GPUs + 2 FPGAs) (preliminary evaluation)



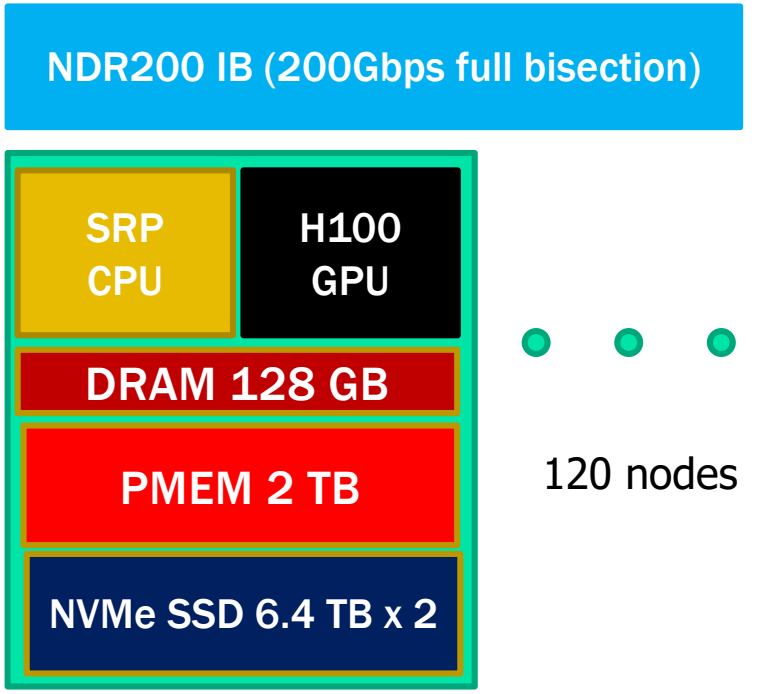
ARGOT for early universe simulation = ARGOT (good for GPU) + ART (good for FPGA)

Timeline of Computing Systems in CCS



OFP2
(2024~)
>150PF

Pegasus: world first combination of PMEM + SPR + H100



120 nodes

Peak performance ~ 6.5PF = 10,000x faster than CP-PACS (#1 in TOP500 Nov. 1996)

OFP2: Oakforest-PACS Ⅱ (tentative name)

- Collaboration with U. Tokyo continues toward highest performance of national university system (Tier-2 of HPCI)
- Up to ~200 PFLOPS peak performance by GPU + CPU
  ⇨ NVIDIA's latest GPU
- Introducing GPU for main performance and CPU-only part still exists for non-GPU application users
- Operation starts from Apr. 2024 ⇨ Later 2024
- RFC will be issued on next month
- GPU-ready code preparation for OFP⇨OFP2 shifting

Development of Novel Scientific Fields

Department of Computational Medical Science

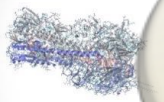
Development of medical technology by computational science in cooperation with medicine, physics, biology, mathematics, data science, and image processing technology.

Leader: Amagasa

Computational Biomolecular Medical Science

Sleep Big Data Analytics & Automatic Sleep Diagnosis

Collaborations: Medicine, Biology, and Physics



Harada

Life Science

Data Science

Computational Medical Science

Computational Media

Computational Physics

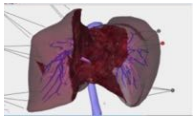
Collaborations: IIIS, C-AIR, CCR

Horie

3DCG Virtual Surgery

Computational Optical Bioimaging

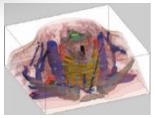
Collaborations: Medicine, Engineering, Design



Shishido

Industry

Collaborations: Biomedical optics, Mathemat



Yajima

Future Plan

- Continuing the codesigning-base supercomputer and application developments
- Cygnus + Pegasus opens the new accelerated supercomputing with large scale memory by cutting edge technologies
- After Oakforest-PACS (OFP) shutdown, follower system (OFP2?) will be introduced on later 2024, under JCAHPC collaboration with Univ. Tokyo
  ⇒ same place with OFP (Kashiwa Campus of Univ. Tokyo)
- CCS continues to grow both in quantity and quality for various fields of computational science and HPC technology
- International collaboration is the key to success