An introduction to Fugaku
–The fastest and most accessible supercomputer-

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NSCC Fugaku Call Briefing Session

The "Fugaku" 富岳 "Exascale" "Applications First" Supercomputer for Society 5.0

Mt. Fuji representing the ideal of supercomputing

High-Peak --- Acceleration of Large Scale Application (Capability)

Broad Base --- Applicability & Capacity
Broad Applications: Simulation, Data Science, AI, …
Broad User Bae: Academia, Industry, Cloud Startups, …
For Society 5.0

Fugaku takes top honors on HPCG and Graph500 June 2020-June 2022 (5 editions in a row)
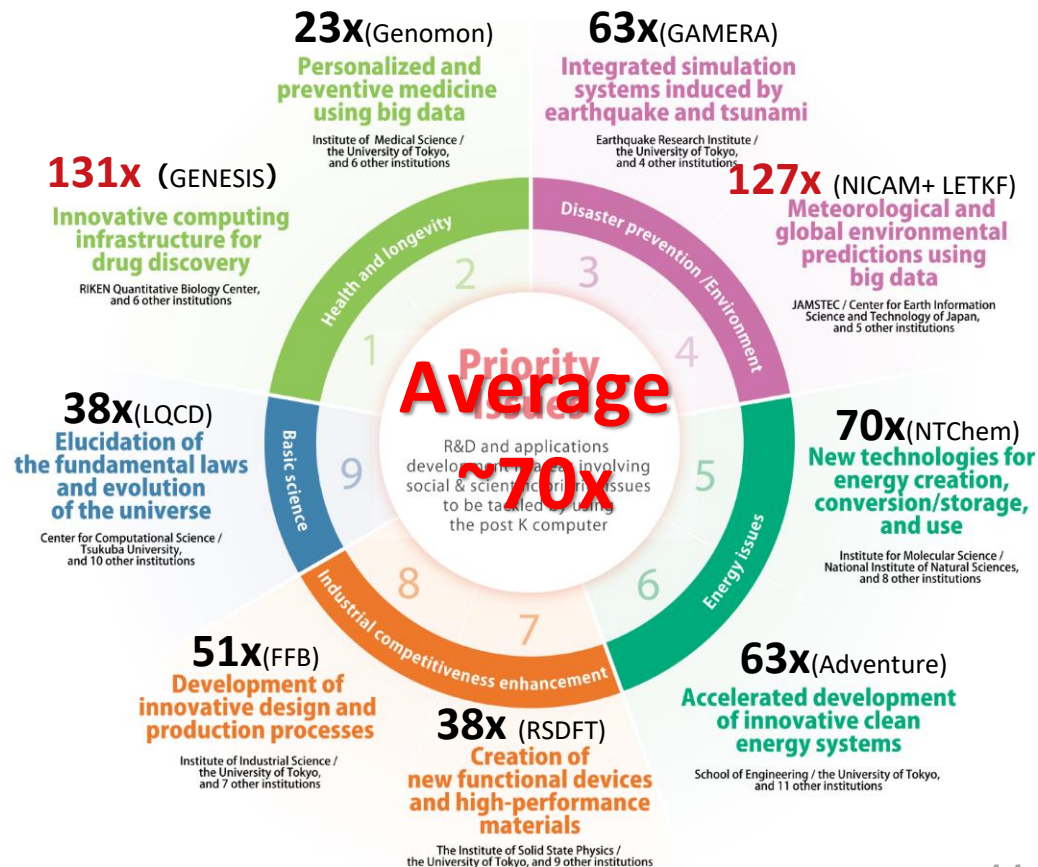
TOP500 (PFLOPS) — *Simulation (Classic)*: 1,102 (USA) / 442.0 (Japan)

HPCG (PFLOPS) — *Simulation (Modern)*: 16.0 (Japan) / 2.93 (USA) — 5.5x

HPL-AI (EFLOPS) — *AI (Deep Learning)*: 6.86 (USA) / 2.0 (Japan)

Graph500 (GTEPS) — *Big Data (Graph Analysis)*: 102,955 (Japan) / 23,756 (China) — 4.3x

ML Perf HPC (CosmoFlow) (models/min) — *Throughput Performance (Deep Learning)* (Nov 2021): 1.29 (Japan) / 0.729 (USA) — 1.77
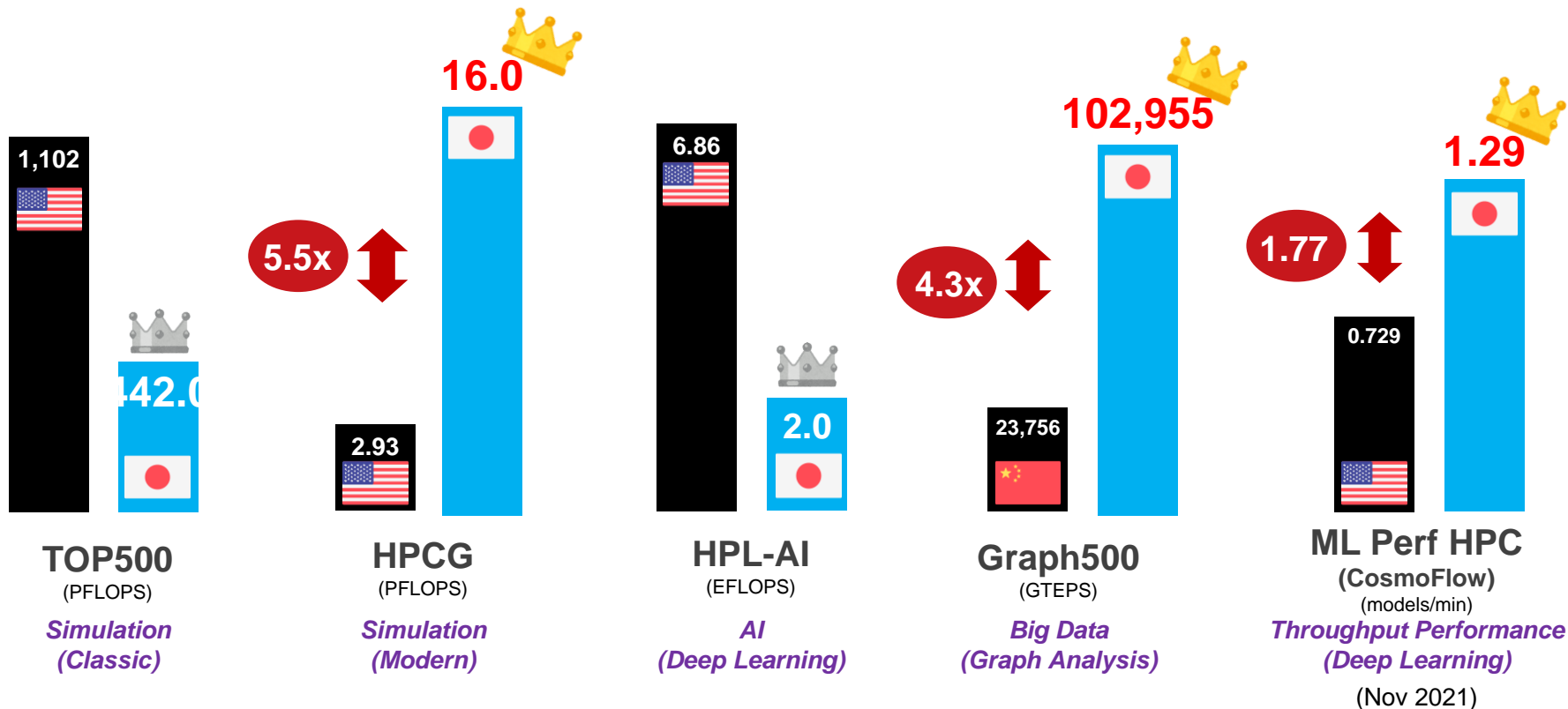
Remains one of the world's top supercomputers 2 years after debut

- **Advanced Applications Co-Design Program to Parallel Fugaku R&D**

- **Select one representative app from 9 priority areas**

  - Health & Medicine

  - Environment & Disaster

  - Energy

  - Materials & Manufacturing

  - Basic Sciences

- **Up to 100x speedup c.f. K-Computer => achieved!**

23x (Genomon)
Personalized and preventive medicine using big data
Institute of Medical Science / the University of Tokyo, and 6 other institutions

63x (GAMERA)
Integrated simulation systems induced by earthquake and tsunami
Earthquake Research Institute / the University of Tokyo, and 4 other institutions

131x (GENESIS)
Innovative computing infrastructure for drug discovery
RIKEN Quantitative Biology Center, and 6 other institutions

127x (NICAM+ LETKF)
Meteorological and global environmental predictions using big data
JAMSTEC / Center for Earth Information Science and Technology of Japan, and 5 other institutions

38x (LQCD)
Elucidation of the fundamental laws and evolution of the universe
Center for Computational Science / Tsukuba University, and 10 other institutions

70x (NTChem)
New technologies for energy creation, conversion/storage, and use
Institute for Molecular Science / National Institute of Natural Sciences, and 8 other institutions

Average ~70x

Priority Issues
R&D and applications development involving social & scientific priority issues to be tackled by using the post K computer

51x (FFB)
Development of innovative design and production processes
Institute of Industrial Science / the University of Tokyo, and 7 other institutions

38x (RSDFT)
Creation of new functional devices and high-performance materials
The Institute of Solid State Physics / the University of Tokyo, and 9 other institutions

63x (Adventure)
Accelerated development of innovative clean energy systems
School of Engineering / the University of Tokyo, and 11 other institutions

Health and longevity
Disaster prevention / Environment
Energy issues
Industrial competitiveness enhancement
Basic science

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MEXT Fugaku Program: Fight Against COVID19
Fugaku resources made available a year ahead of general production
(more research topics under international solicitation, also joined US-lead COVID-19 High Performance Computing Consortium)

Medical-Pharma

*Prediction of conformational dynamics of proteins on the surface of SARS-Cov-2*
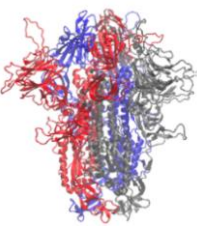
GENESIS MD to interpolate unknown experimentally undetectable dynamic behavior of spike proteins, whose static behavior has been identified via Cryo-EM

（（Yuji Sugita, RIKEN）

Fragment molecular orbital calculations for COVID-19 proteins

Large-scale, detailed interaction analysis of COVID-19 using Fragment Molecular Orbital (FMO) calculations using ABINIT-MP
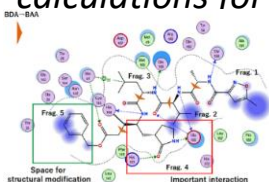
(Yuji Mochizuki, Rikkyo University)
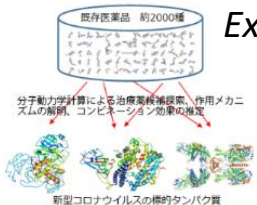
Exploring new drug candidates for COVID-19

Large-scale MD to search & identify therapeutic drug candidates showing high affinity for COVID-19 target proteins from 2000 existing drugs

(Yasushi Okuno, RIKEN / Kyoto University)

Host genetic analysis for severe COVID-19

Whole-genome sequencing of severe cases of COVID-19 and mild or asymptomatic infections, and identify risk-associated genetic variants for severe disease

(Satoru Miyano, Tokyo Medical and Dental University)
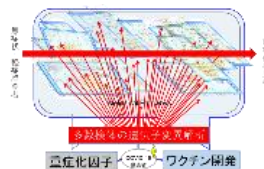
Societal-Epidemiology

Prediction and Countermeasure for Virus Droplet Infection under the Indoor Environment

Massive parallel simulation of droplet s... and hat tr... environme... trains, offi... hospital r...

2021 ACM Gordon Bell Prize

(M... ...e University)

Simulation analysis of pandemic phenomena

Combining simulations & analytics of disease propagation w/contact tracing apps, economic effects of lockdown, and reflections social media, for effective mitigation policies

（Nobuyasu Ito, RIKEN）

Spec

Instruction set architecture	Armv8.2-A SVE 512 bit Fujitsu extension: hardware barrier, sector cache, prefetch
Number of core	48 + 2 assistant cores 4 CMG (Core Memory Group, NUMA node)
Performance Normal mode (CPU clock speed: 2 GHz)	Double precision: 3.072 TF; single precision: 6.144 TF; half-precision: 12.288 TF
Performance Boost mode (CPU clock speed: 2.2 GHz)	Double precision: 3.3792 TF; single precision: 6.7584 TF; half-precision: 13.5168 TF
Cache *1 *2	L1D/core: 64 KiB, 4way, 256 GB/s (load), 128 GB/s (store) L2/CMG: 8 MiB, 16way L2/node: 4 TB/s (load), 2 TB/s (store) L2/core: 128 GB/s (load), 64 GB/s (store)
Memory	HBM2 32 GiB, 1024 GB/s
Interconnect	Tofu Interconnect D (28 Gbps x 2 lane x 10 port)
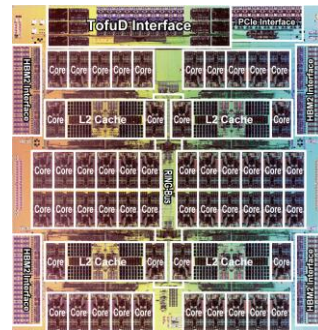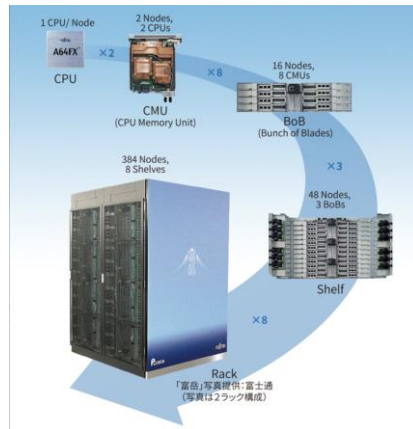
CPU-Die (Image courtesy of Fujitsu)

https://www.r-ccs.riken.jp/en/fugaku/about/

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Software stack

Programming environment

Compiler	Fortran 2008 and Fortran 2018 C11 with GNU and Clang extensions C++14 and C++17 with GNU and Clang extensions OpenMP 4.5 and OpenMP 5.0 Java
Parallel programing	XcalableMP [Details of XcalableMP (PDF 535 KB)] FDPS [Details of FDPS (PDF 260 KB)]
Script language	Python / Numpy / Scipy, Ruby
Numerical library	BLAS, LAPACK, ScaLAPACK SSL II (Fujitsu) EigenExa, Batched BLAS, 2.5D-PDGEMM

System software

Open-source management tool	Spack [Details of Spack (PDF 355 KB)]
Container, virtual machine	Singularity, KVM
OS	Red Hat Enterprise Linux 8 McKernel [Details of McKernel (PDF 641 KB)]
MPI	Fujitsu MPI (Based on OpenMPI), MPICH-Tofu (Based on MPICH) [Details of MPICH-Tofu (PDF 404 KB)]
File IO	LLIO DTF (Data Transfer Framework) [Details of DTF (PDF 220 KB)]

https://www.r-ccs.riken.jp/en/fugaku/about/

OSS apps Performance

OSS Application Performance on FX1000/FX700
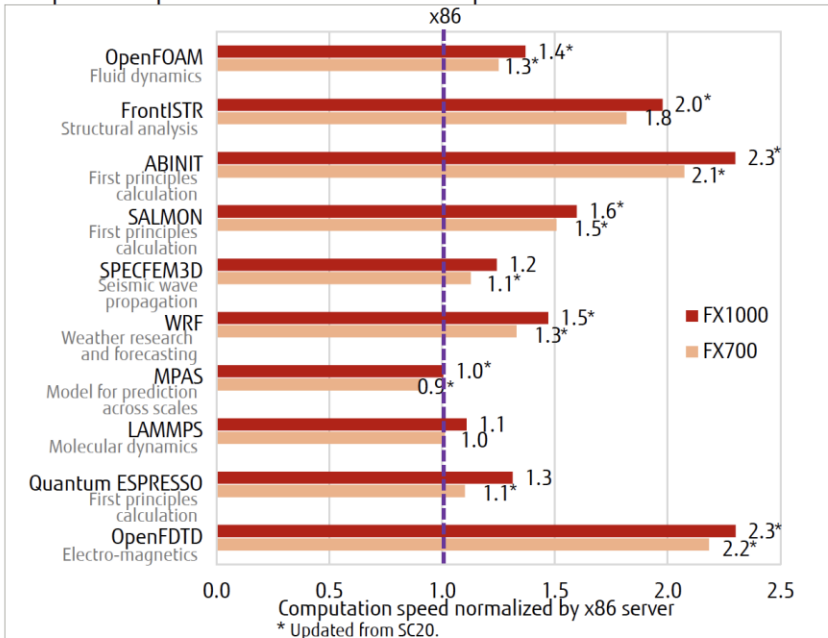
Fujitsu in ISC21
https://www.fujitsu.com/downloads/SUPER/topics/isc21/applications-for-primehpc.pdf

Commercial software

Commercial Applications List — FUJITSU

- Availability of commercial applications for FX1000.
  Several applications were already verified on Fugaku.

Categories	Applications	Vendors	Availability	Notes
Engineering (Fluid dynamics)	CONVERGE	Convergent Science (East Asia distributor : IDAJ Co., LTD.)	Available in 3Q '21	Solver components only Verified on Fugaku
	Cradle CFD | scFLOW	Software Cradle Co., Ltd.	Beta ver. in 3Q '21	Verified on Fugaku
	Fluent	Ansys, Inc.	Alpha ver. in July '21	Solver components only
	HELYX	ENGYS Ltd.	Plan to be available *	
	Simcenter STAR-CCM+	Siemens Digital Industries Software, Inc.	Plan to be available *	
Engineering (Structural analysis)	ESI Virtual Performance Solution (VPS)	ESI Group	Available in 3Q '21	Explicit features only Verified on Fugaku
	LS-DYNA	Ansys, Inc.	**Available**	Verified on Fugaku
Engineering (Electromagnetics)	JMAG	JSOL Corporation	Plan to be available *	Verified on Fugaku
	Poynting	Fujitsu Limited	**Available**	Verified on Fugaku
Chemistry	Amber	University of California, San Francisco	**Available**	Collaboration with Australian National University
	Gaussian16	Gaussian, Inc.	**Available**	
Others	NAG Fortran Compiler	Numerical Algorithms Group Ltd	Available for FX700	Will be verified for FX1000 on customer request

*Release date will be announced later. **All application names used in this slide are trademarks or registered trademarks of their respective venders.

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Will be available in 11/21

Fujitsu in ISC21
https://www.fujitsu.com/downloads/SUPER/topics/isc21/applications-for-primehpc.pdf

Most of the other software will be available till the end of March.

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login nodes and servers for pre-post processing

Fugaku users can use them with no-charge

Name	arch	# of core /node	Memory capacity	# of server	GPU
Login node	Intel	16x2	96/192GB	8	N/A
	Arm(TX2)	28x2	96GB	4	N/A
Login node with large memory	Intel	16x2	6,144GB	2	N/A
Visualization server	Intel	12x2	192GB	8	V100x2/node
Cloud storage gateway	Intel	16x2	256GB	2	N/A
Virtual Pre-Post server	Intel	26x2	384GB	30	N/A

Open On Demand for Fugaku is now available
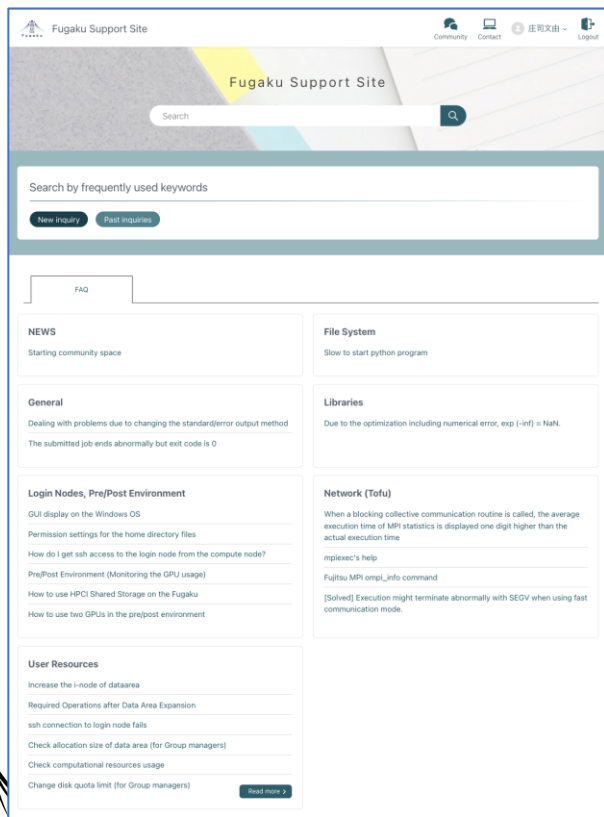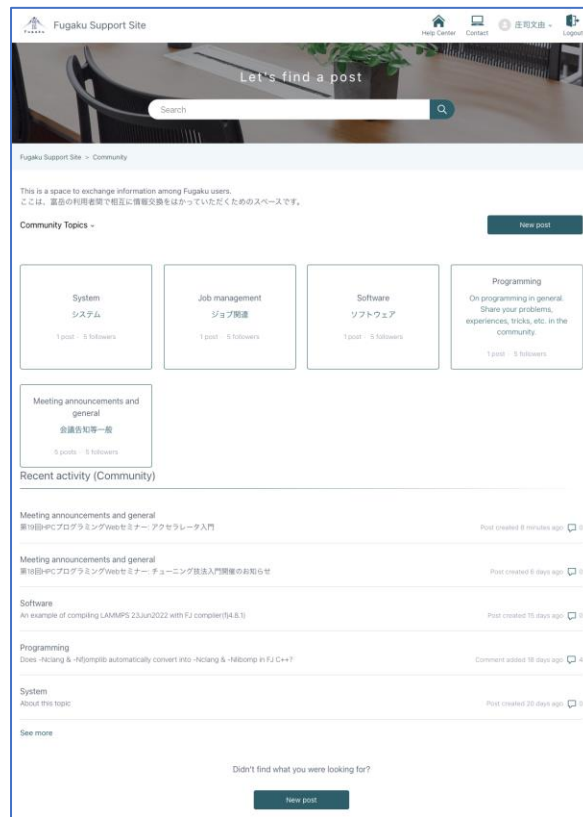
Helpdesk/User Forum powered by Zendesk

Helpdesk/FAQ

User Forum

Events for tuning technique promotion for A64FX

- Objective

  - To promote tuning technique for A64FX as quickly and widely as possible.

- Policy

  - Experts who have experience of tuning of large scale simulation on Fugaku introduce and share their technique and experience.

  - Materials and talks are in English and everything is recorded and opened.

  - Online based meeting and anyone (even non-Fugaku user) can join the meeting.

  - Organized by RIST and R-CCS

- Pointers for past meetings

  - https://www.hpci-office.jp/pages/e_meetings_A64FX

  - Slack workspace: https://join.slack.com/t/meetingforapp-16k4753/shared_invite/zt-ms93bjpy-BOGm1bvDsTTSJd5bsWL18g

Meeting	Date	Topics
The first meeting for application code tuning on A64FX computer systems	December 9, 2020	Performance tuning of Graph500 benchmark on Supercomputer Fugaku A64FX Tuning - SCALE on Fugaku -
The second meeting for application code tuning on A64FX computer systems	December 23, 2020	LQCD tuning on A64FX Optimization of GENESIS on Fugaku
The 3rd meeting for application code tuning on A64FX computer systems	February 3, 2021	Development of Massively Parallel DMRG for Fugaku HPL-AI bechmark on Fugaku
The 4th meeting for application code tuning on A64FX computer systems	March 17, 2021	Development of EigenExa from K to Fugaku, and beyond Fugaku Development of a deep neural network library for A64FX
The 5th meeting for application code tuning on A64FX computer systems	April 27, 2021	Performance tuning on LAMMPS for A64FX system CPU and Thread Parallelization Tuning of FFVHC-ACE on Fugaku
The 6th meeting for application code tuning on A64FX computer systems	June 30, 2021	Overview of Software Environment on Fugaku VELOC: Very Low Overhead Checkpointing System Hands-on session on VELOC
The 7th meeting for application code tuning on A64FX computer systems	January 27, 2022	Basic Performance of File system on Fugaku Basic Performance of Fujitsu MPI on Fugaku
The 8th meeting for application code tuning on A64FX computer systems	April 28, 2022	performance tuning and analysis for the axhelm kernel in NeKS000/RS CFD codes Performance tuning of N-body kernel for A64FX processor
The 9th meeting for application code tuning on A64FX computer systems	July 27, 2022	Examples of serial-code optimization for A64FX processor cores Porting and optimizing GROMACS on Fugaku
The 10th meeting for application code tuning on A64FX computer systems	November 9, 2022	Performance tuning of MLPerf HPC benchmark on Fugaku FFT libraries on Fugaku

Summary

- **Fugaku is a general-purpose supercomputer**

  - consisting of an Arm-based CPU only (no accelerators)

  - developed by co-design of computer and computational scientists

- **Fugaku provides not only high-end computing capability but also high usability.**

  - Software eco-system for Arm-based architecture

  - Many optimized OSS/ISV software has already been available, and Spack helps to use them easily.

  - Rich helpdesk/FAQ support and User Forum platform will be useful if you face a problem with Fugaku usage.

We look forward to serving Fugaku to all of you

Thank you very much for your attention