SESSION: SOFTWARE PRODUCTION AND INTEGRATION

Virtual Fugaku bridging supercomputers and Clouds

InPEx 2025

April 15, 2025

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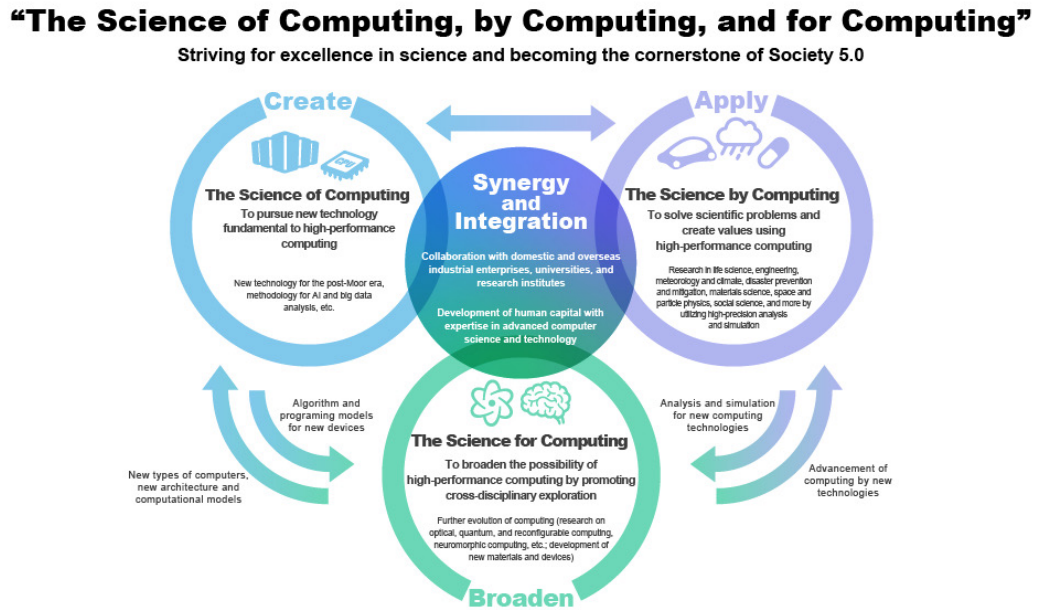
Acknowledgement: Some of the sentences and the figures are created by chatGPT

RIKEN Center for Computational Science (RIKEN R-CCS)

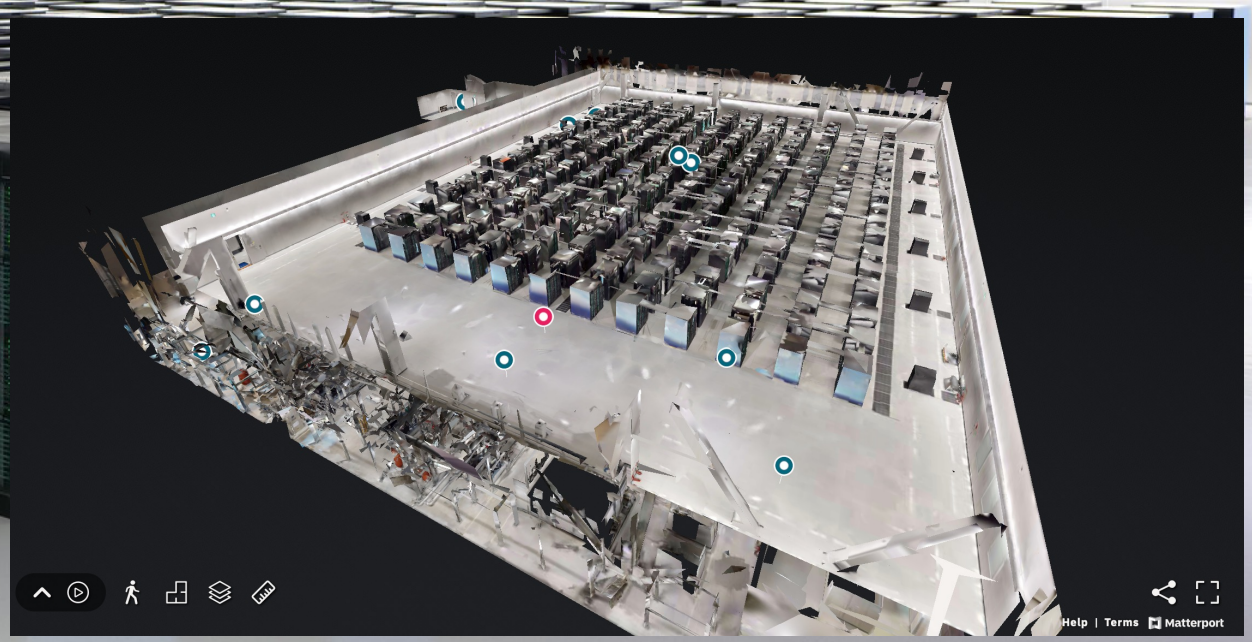
- **RIKEN R-CCS is one of 13 RIKEN strategic research and infrastructure centers**
- **Mission in R-CCS:**
  - Conduct the state-of-the-art research that integrates “simulation,” “big data analysis,” and “AI” through high performance computing (HPC) to solve scientific and social issues and revolutionize society
- **Three R&D thrusts in R-CCS:**
  - Cultivate the future through “Science of computing, by computing, and for computing”
  - Integrate Computational Science, Data Science, and AI
  - Aim to Solve Issues for Advanced Modern Society



「富岳」Supercomputer Fugaku

Peak Performance	Normal Mode: 2.0 GHz	488 PFLOPS (FP64) 977 PFLOPS (FP32) 1.95 EFLOPS (FP16) 3.90 EOPS (INT8)
	Boost Mode: 2.2 GHz	537 PFLOPS (FP64) 1.07 EFLOPS (FP32) 2.15 EFLOPS (FP16) 4.30 EOPS (INT8)
Total Memory		4.85 PiB
Total Memory Bandwidth		163 PB/s

Fugaku 3D Vritual Tour

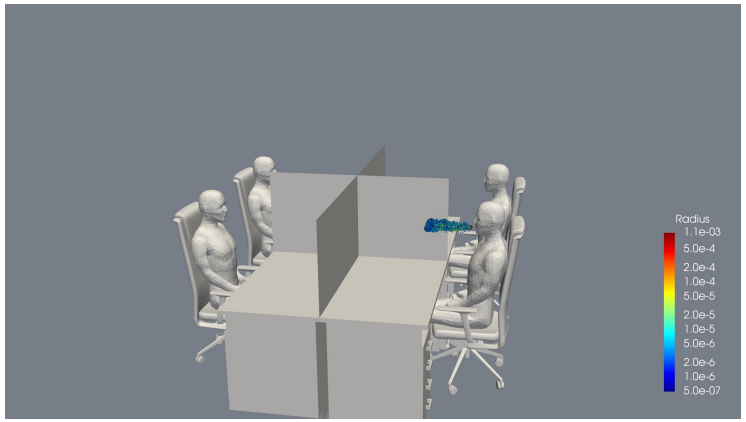


Major achievements of Fugaku

#1 in major benchmark rankings:
TOP500 and HPL-AI (Jun.2020-Nov.2021),
Graph500 and HPCG (Jun.2020-)

#1 in MLPerf HPC(Nov.2021-)

ACM Gordon Bell Special Prize for HPC based COVID-19 research(Nov.2021), also 2022



Weather forecasting trial for “guerrilla downpour” in TOKYO2020 Olympic/Paralympic games

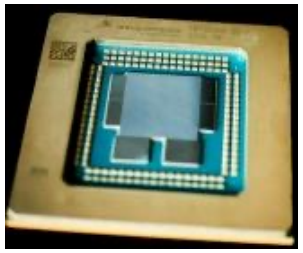
今回の実証実験で表示される「3D雨雲ウォッチ」アプリイメージ

Virtual Fugaku:
MoU Between AWS & R-CCS (Effective: January 2023)

- **RIKEN R-CCS has been advancing usability of Fugaku to facilitate the collaboration**
  → Expanding the Scientific Platforms of Fugaku to the AWS Cloud

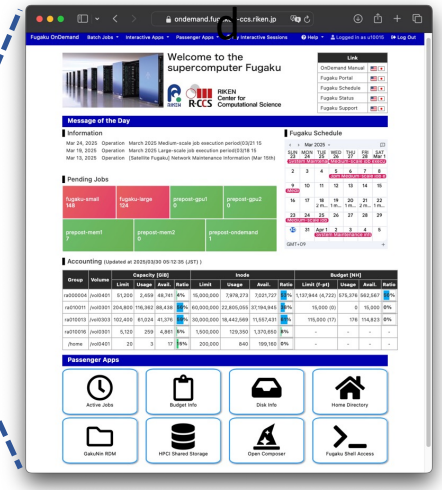
- **Compatible ISA in Arm eco-system**
  - Fugaku (by Fujitsu/RIKEN): A64FX HPC (Arm+SVE CPU), 2018
  - AWS (by Amazon): AWS Graviton3/3E (Arm+SVE CPU), 2022
- → Applications are compatible on both Fugaku and AWS


A64FX


Graviton3

- **Virtual Fugaku platform**
  - Common interface provided on Fugaku and AWS
  - Users can enjoy computational power of both Fugaku and AWS through the same interface

Open OnDeman

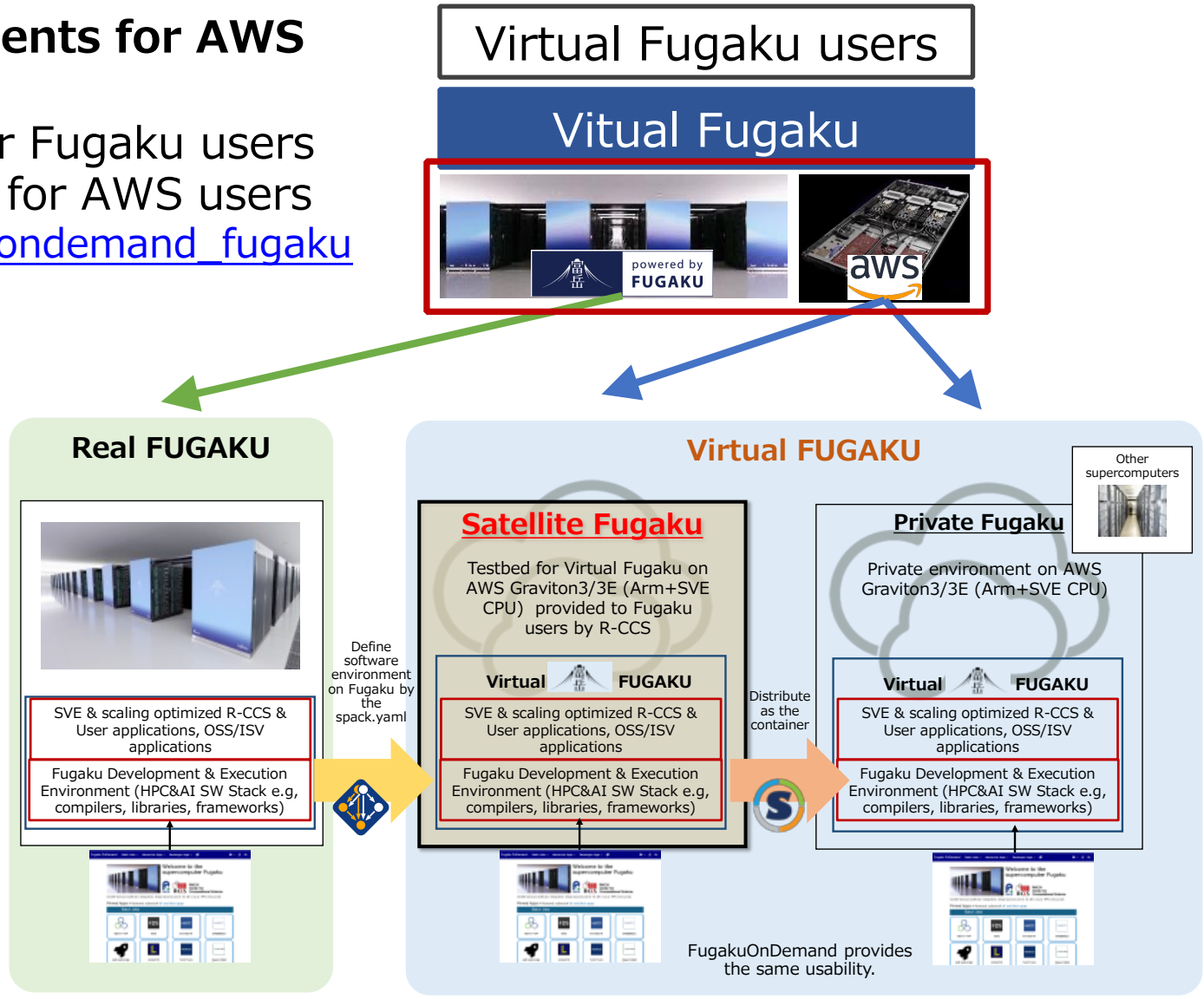


Virtual Fugaku enables gradual software/application dev.

- **Virtual Fugaku provides two environments for AWS Graviton CPUs:**
  - Satellite Fugaku: A test environment for Fugaku users
  - Private Fugaku: A Singularity container for AWS users
    - Github: https://github.com/RIKEN-RCCS/ondemand_fugaku

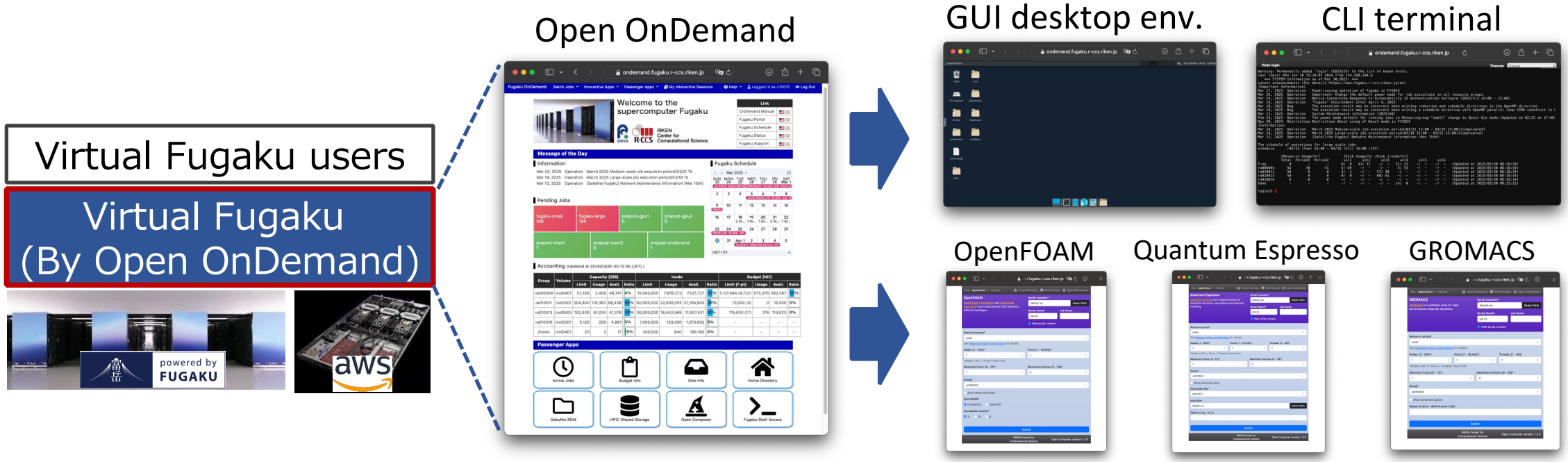
- **Both environments share the same software configuration**
  - Defined and containerized by Spack*
  - *Spack: a package mgmt. tool
- **Enables gradual software/application development**
  - E.g., Companies develop methods using massive Fugaku resource, conduct production run on AWS or private cloud

→ Allows immediate propagation of latest research results onto production



Virtual Fugaku provides web portal powered by Open OnDemand

- **Open OnDemand is web portal for HPC clusters**
  - Developed mainly by the Ohio State University
  - Open-source software used by over 250 institutions worldwide
- **Use HPC systems from user's web browser**
  - No other software installation required
  - File upload/download, job submission, use of applications/services and monitoring by browser
- **Multi-level applications/services provision**
  - PaaS: GUI desktop, CLI terminal
  - SaaS: Many scientific applications, data services, develop env., visualization tools and others



Supported Applications/Serivices in Virtual Fugaku (Release: Aug. 8, 2024))

- **Virtual Fugaku supports a wide variety of applications and servicies**
  - Interactive applications

Category	Application
Development	Remote Desktop, JupyterLab, MATLAB, RStudio, VSCode
Profiler	NVIDIA Visual Profiler, NVIDIA Nsight Compute*, NVIDIA Nsight Systems, Vampir
Viewer	AVS/Express, C-Tools, GaussView, ImageJ, OVITO, Paraview, PyMOL, SALMON view, Smokeview, VESTA, VMD, VisIt, XCrySDen
Workflow	WHEEL

  - Batch-based applications

Category	Application
Climate	SCALE
Computer Aided Engineering	FDS, FrontFlow (blue/X), FrontISTR, OpenFOAM (Foundation/OpenCFD)
Condensed Matter Physics	ALAMODE, AkaiKKR, HΦ, mVMC, OpenMX, PHASE/0, Quantum Espresso, SALMON
Molecular Dynamics	GENESIS, GROMACS, LAMMPS, MODYLAS
Quantum Chemistry	ABINIT-MP, Gaussian, NTChem, SMASH
Quantum Simulation	braket

RIKEN R-CCS keeps upgrading the virtual Fugaku platform to advance usability of supercomputers and the clouds and facilitate international collaborations

Recent News & Future Plans for Virtual Fugaku

- **News on April 2025**
  - Includes pre-installed CFD application (ANSYS Fluent)
  - Available as a Singularity container image (v1.2): https://cloud.sylabs.io/library/riken-rccs/virtual-fugaku/vf-ver1.2
  - Accompanied by an open-source workflow tool: OpenComposer on GitHub: https://github.com/RIKEN-RCCS/OpenComposer

- **Future Plans**
  - Hybrid HPC environment with Virtual Fugaku (Common software stack)
    - Provide the Virtual Fugaku image for other environments (e.g. x86, GPU).
    - Apply to new R-CCS Systems, including AI for science and Quantum-HPC Hybrid Platforms
  - Expand, maintain, and update software packages continuously.
    - Keep up with emerging technologies, AI frameworks, and ML software
    - Most frequently used software in Fugaku.
    - Implement CI/CD/CT processes.
  - Further improve usability
    - Allow on-demand private packaging based on a Spack's feature of build caches.