

Application Software Provisioning toward Supercomputer "Fugaku"

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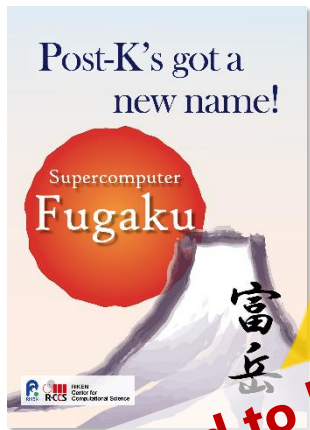
Research Organization for Information Science & Technology



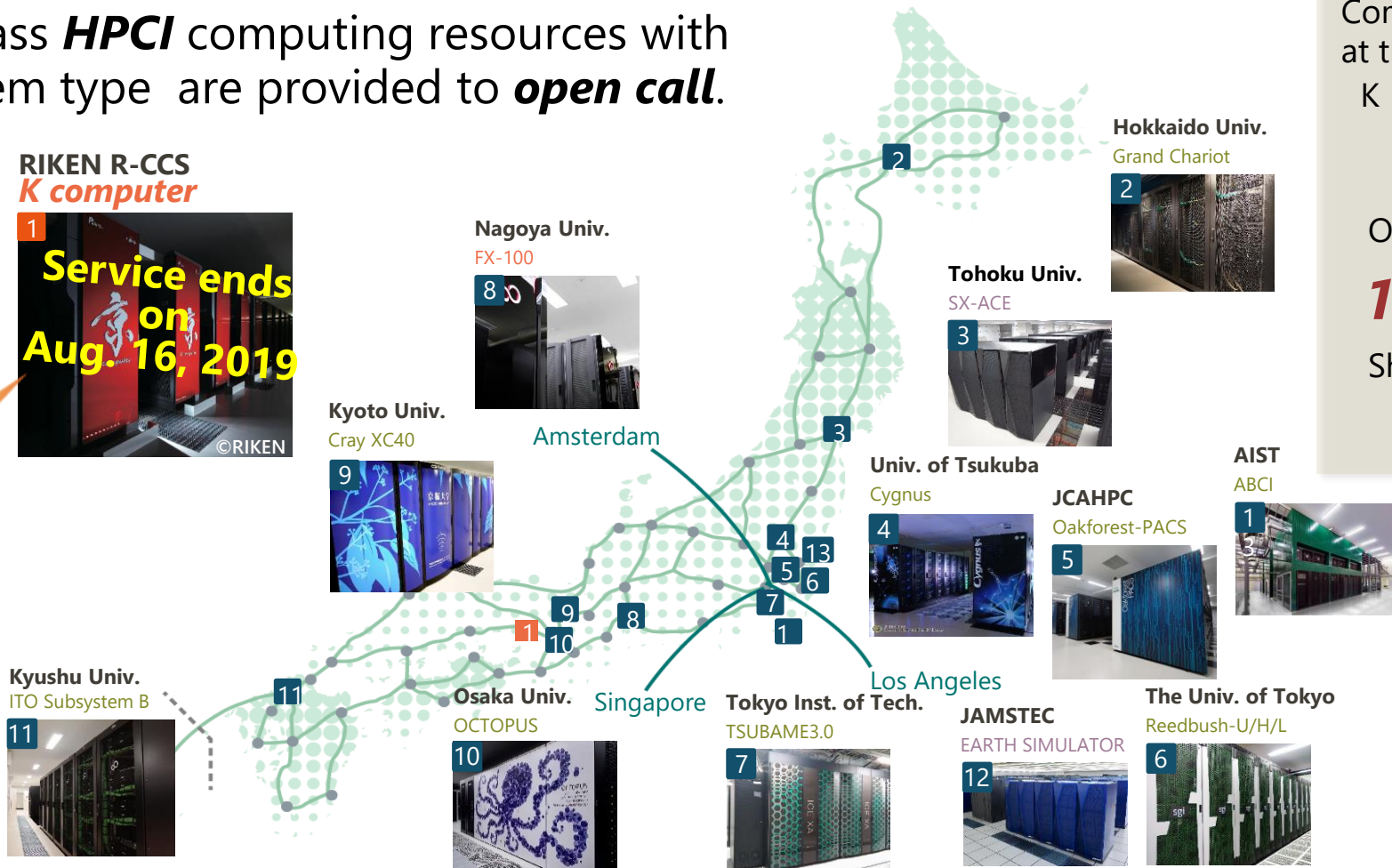
June 13, Arm HPC User Group, ISC 2019

HPCI and Supercomputer Fugaku

- **HPCI, High Performance Computing Infrastructure** established in 2012 as national HPC infrastructure, is a system connecting the Tier 0 flagship system and part of the Tier 1 major Universities and National Lab systems by high speed academic network (SINET-5).
- World's top class **HPCI** computing resources with variety of system type are provided to **open call**.



Scheduled to be operational around 2021



Computing resources allocated at the Public Call in FY 2019
K computer

1.5 PFlops x Year

Other HPCI machines in total

14.2 PFlops x Year

Shared Storage

45 PB

SINET-5 (100 Gbps)

- : node
- : domestic line
- : international line

As of June 2019

- Fujitsu adopts Arm ISA and develops own micro architecture with HPC enhancement

<http://www.fujitsu.com/jp/Images/20180821hotchips30.pdf>

A64FX Chip Overview

■ Architecture Features

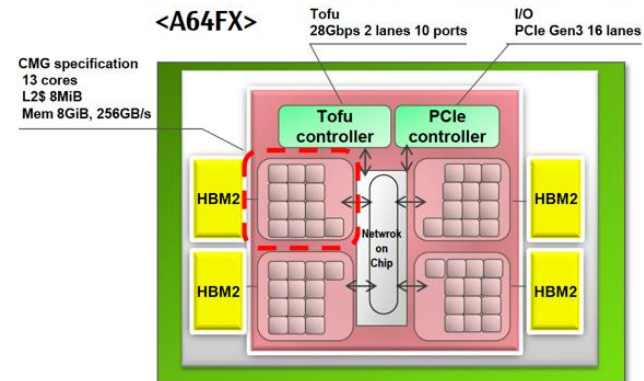
- Armv8.2-A (AArch64 only)
- SVE 512-bit wide SIMD
- 48 computing cores + 4 assistant cores*
*All the cores are identical
- HBM2 32GiB
- Tofu 6D Mesh/Torus 28Gbps x 2 lanes x 10 ports
- PCIe Gen3 16 lanes

■ 7nm FinFET

- 8,786M transistors
- 594 package signal pins

■ Peak Performance (Efficiency)

- >2.7TFLOPS (>90%@DGEMM)
- Memory B/W 1024GB/s (>80%@Stream Triad)



| | A64FX (Post-K) | SPARC64 Xlfx (PRIMEHPC FX100) |
|------------------|----------------|-------------------------------|
| ISA (Base) | Armv8.2-A | SPARC-V9 |
| ISA (Extension) | SVE | HPC-ACE2 |
| Process Node | 7nm | 20nm |
| Peak Performance | >2.7TFLOPS | 1.1TFLOPS |
| SIMD | 512-bit | 256-bit |
| # of Cores | 48+4 | 32+2 |
| Memory | HBM2 | HMC |
| Memory Peak B/W | 1024GB/s | 240GB/s x2 (in/out) |

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CPU : ~2.7TFLOps (x ~20 of K)

1 rack : ~1PFlops (x ~80 of K)

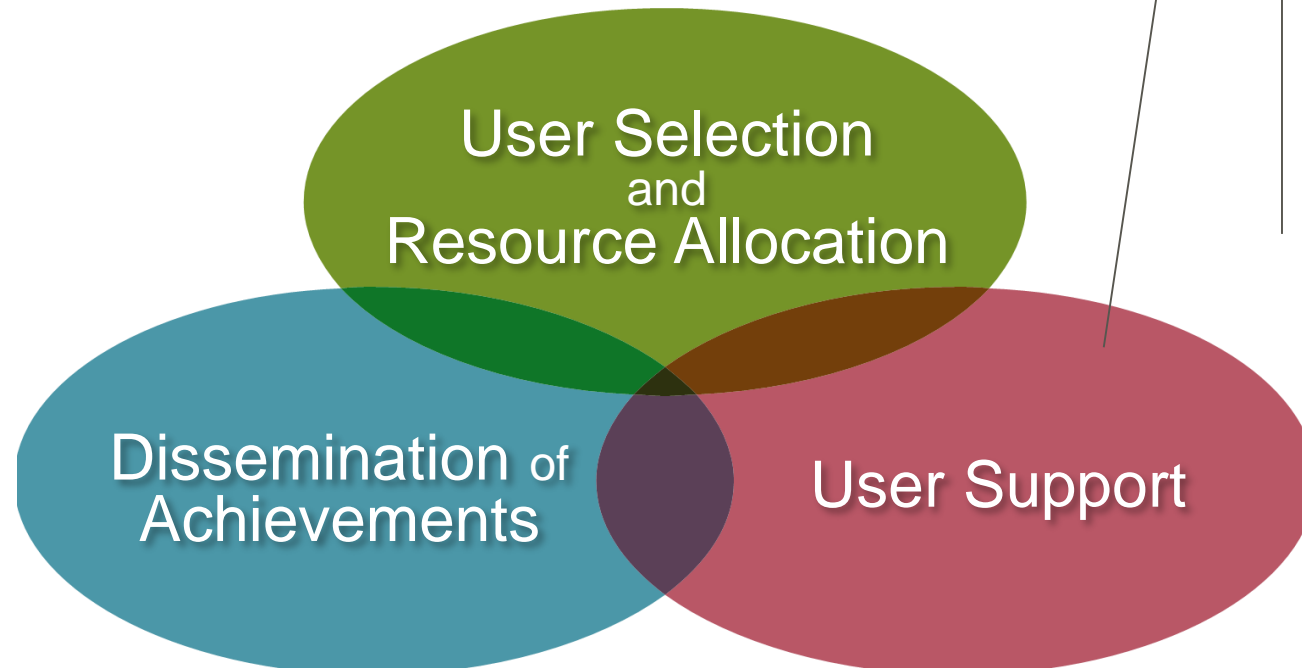


~10 racks

■ RIST's Roles

- ◆ Registered Institution for Facilities Use Promotion of the "Specific High-speed Computer Facilities" (K computer)
- ◆ Representative for HPCI Operation

■ RIST's Activities



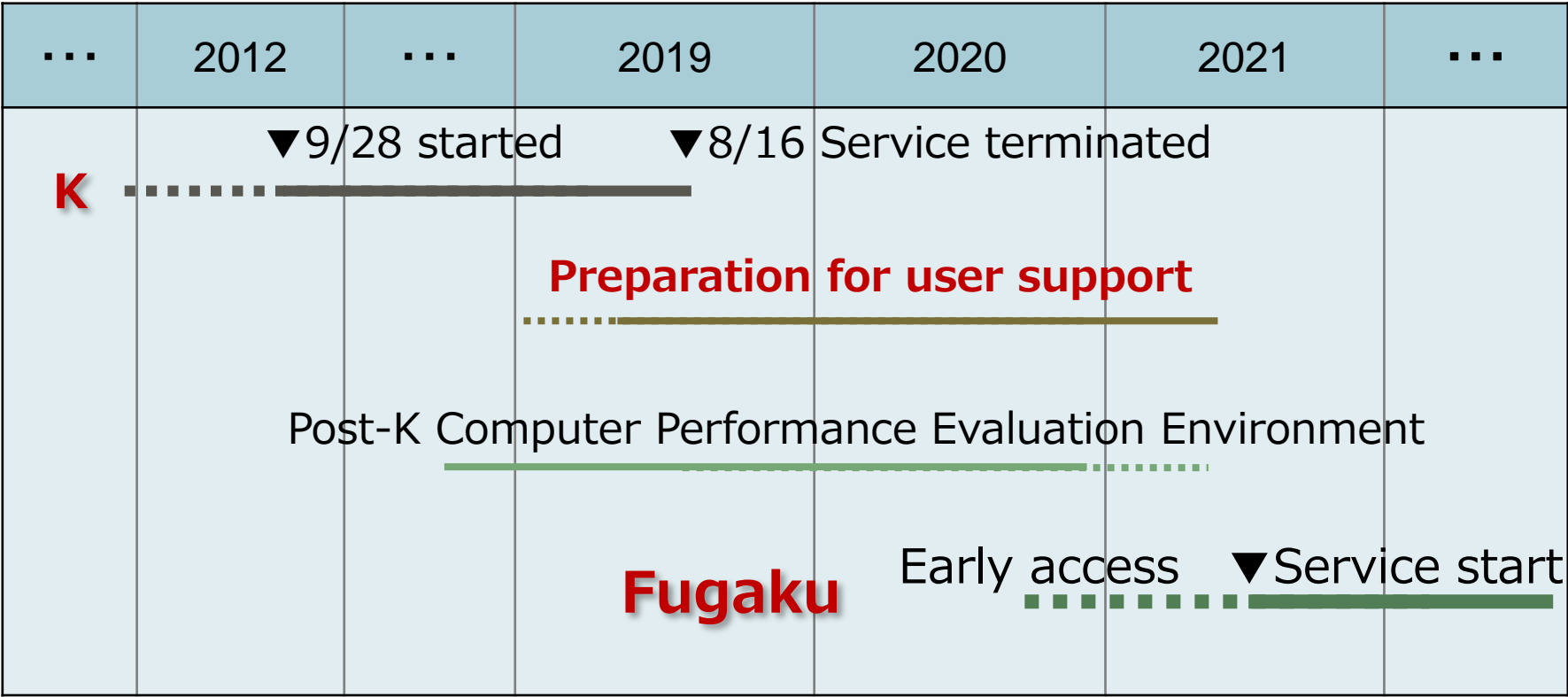
First Level Support

Advanced Level Support

- ◆ User application porting
- ◆ Serial and scalability tuning
- ◆ Application software provisioning

We are undertaking user support activities toward Fugaku.

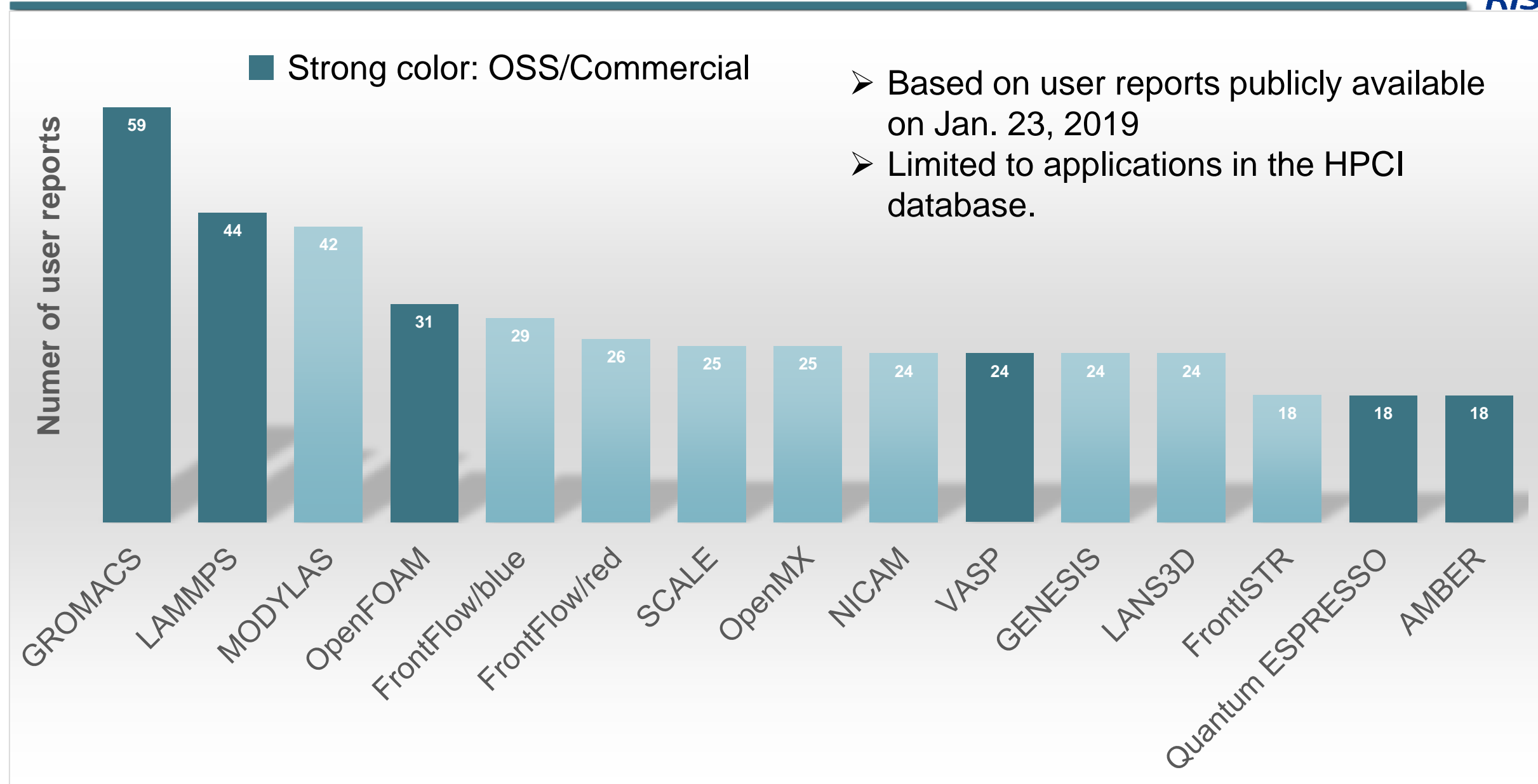
- Toward user support for Fugaku
 - ◆ Preparation for application software provisioning on Fugaku
 - ◆ Upskilling of the support team for tuning supports on Fugaku
 - ◆ Preparation for education program about utilization of Fugaku



Application Software Provisioning

for efficient utilization
of HPCI supercomputers

Widely-used Applications in HPCI projects



- Various kinds of software are **ready-to-use** for HPCI users now, collaborating with computing centers associated with HPCI, and National Projects
 - ◆ Widely-used **open-source software (OSS)**
 - ◆ Promising **software developed by JP National Projects (NP)**

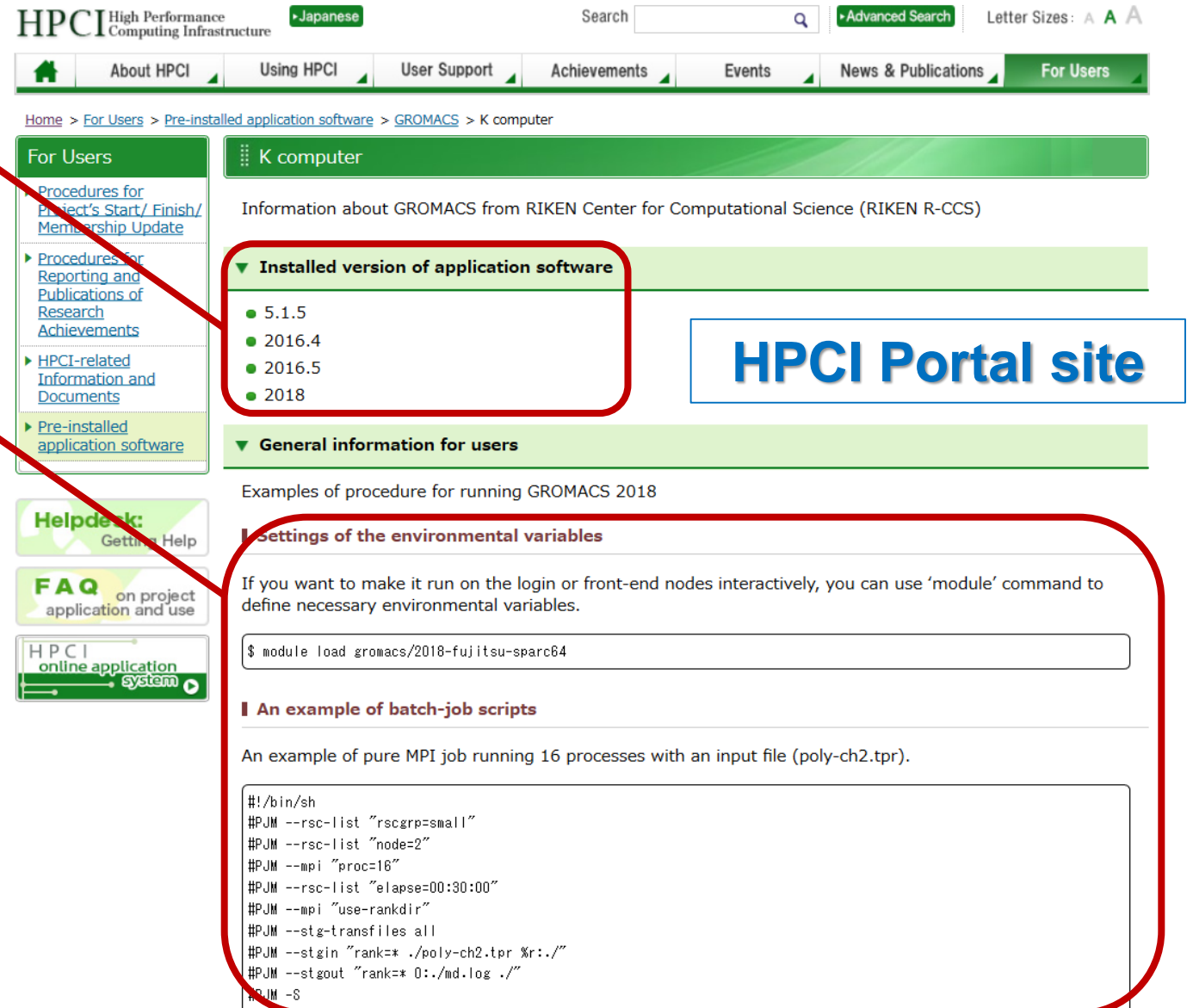
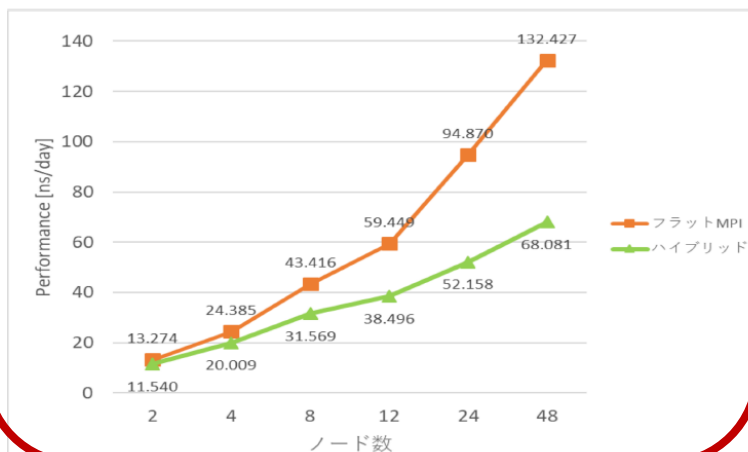
| Kinds | Application software | Installed machines |
|-------|--|--------------------------------|
| OSS | OpenFOAM, LAMMPS, Quantum ESPRESSO, GROMACS | ■ K ■ FX100 (in HPCI sytem) |
| NP | NTChem, MODYLAS, SMASH, OpenMX, SALMON, HΦ, GENESIS, ABINIT-MP, PHASE/0, FrontFlow/blue, FrontISTR | ■ HPCI other than K |

What ready-to-use means?

Ready-to-use means

- ◆ Pre-installation of the software
- ◆ Documents for Utilization
 - Examples for utilization
 - Tutorial
 - Benchmark information

GROMACS 2018.3 d.poly-ch2 (6,000 (12,000) atoms, 5,000 steps)



HPCI Portal site

Home > For Users > Pre-installed application software > GROMACS > K computer

For Users

- Procedures for Project's Start/ Finish/ Membership Update
- Procedures for Reporting and Publications of Research Achievements
- HPCI-related Information and Documents
- Pre-installed application software

Installed version of application software

- 5.1.5
- 2016.4
- 2016.5
- 2018

General information for users

Examples of procedure for running GROMACS 2018

Settings of the environmental variables

If you want to make it run on the login or front-end nodes interactively, you can use 'module' command to define necessary environmental variables.

```
$ module load gromacs/2018-fujitsu-sparc64
```

An example of batch-job scripts

An example of pure MPI job running 16 processes with an input file (poly-ch2.tpr).

```
#!/bin/sh
#PJM --rsc-list "rscgrp=small"
#PJM --rsc-list "node=2"
#PJM --mpi "proc=16"
#PJM --rsc-list "elapsed=00:30:00"
#PJM --mpi "use-rankdir"
#PJM --stg-transfiles all
#PJM --stgin "rank=* ./poly-ch2.tpr %r:./"
#PJM --stgout "rank=* 0:./md.log ./"
#PJM -S
```

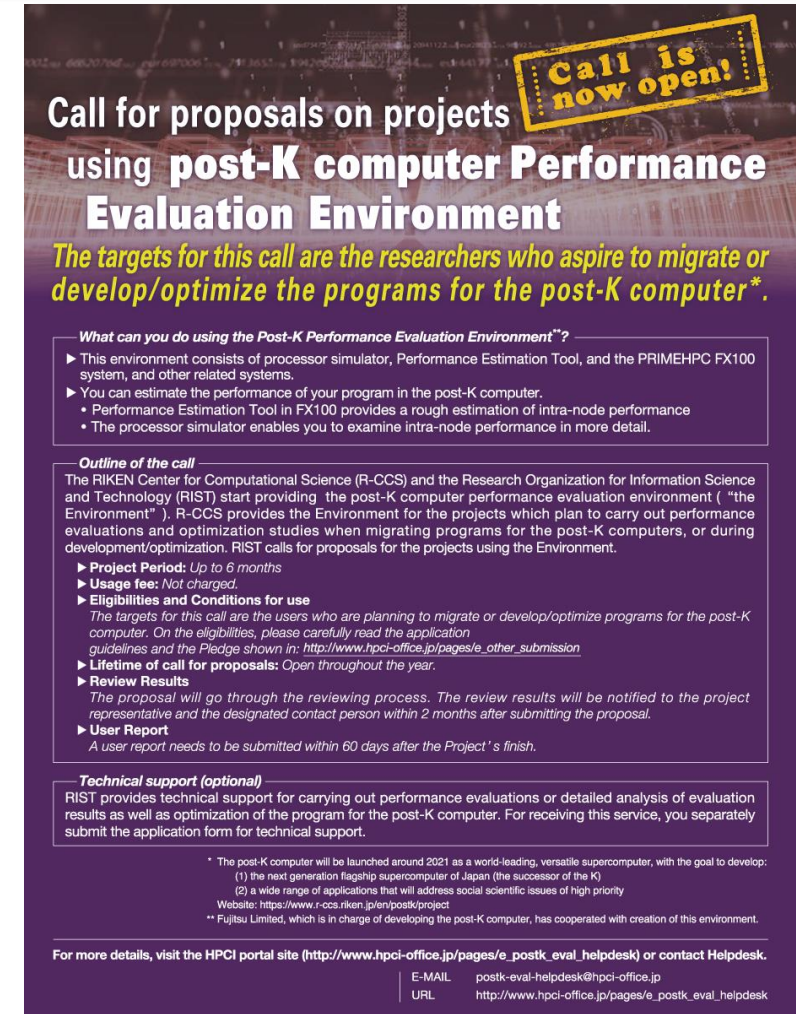
RIST is currently undertaking

Application Software Provisioning for Fugaku,
looking ahead to the future collaboration with Arm community.

Call for project proposals Post-K Computer Performance Evaluation Environment

*Estimate your code performance
on future Supercomputer Fugaku !*

- Who are the targets?
 - ◆ Potential users of **Fugaku**
- What can you do with the Environment?
 - ◆ Approximate performance of programs is attainable
 - ◆ The Environment mainly consists of:
 - “Processor simulators”
 - “Performance Estimation Tools” (on FX100)
 - “Compilers (Fortran, C/C++)” for **Fugaku**
- Call for project proposals now open
 - ◆ The project period is **up to 6 months**
 - ◆ The call is **open throughout the year**
 - ◆ **RIST provides technical supports**



**Call for proposals on projects
using post-K computer Performance
Evaluation Environment**

The targets for this call are the researchers who aspire to migrate or develop/optimize the programs for the post-K computer.*

What can you do using the Post-K Performance Evaluation Environment?**

- ▶ This environment consists of processor simulator, Performance Estimation Tool, and the PRIMEHPC FX100 system, and other related systems.
- ▶ You can estimate the performance of your program in the post-K computer.
 - Performance Estimation Tool in FX100 provides a rough estimation of intra-node performance
 - The processor simulator enables you to examine intra-node performance in more detail.

Outline of the call

The RIKEN Center for Computational Science (R-CCS) and the Research Organization for Information Science and Technology (RIST) start providing the post-K computer performance evaluation environment (“the Environment”). R-CCS provides the Environment for the projects which plan to carry out performance evaluations and optimization studies when migrating programs for the post-K computers, or during development/optimization. RIST calls for proposals for the projects using the Environment.

- ▶ **Project Period:** Up to 6 months
- ▶ **Usage fee:** Not charged.
- ▶ **Eligibilities and Conditions for use**
The targets for this call are the users who are planning to migrate or develop/optimize programs for the post-K computer. On the eligibilities, please carefully read the application guidelines and the Pledge shown in: http://www.hpci-office.jp/pages/e_other_submission
- ▶ **Lifetime of call for proposals:** Open throughout the year.
- ▶ **Review Results**
The proposal will go through the reviewing process. The review results will be notified to the project representative and the designated contact person within 2 months after submitting the proposal.
- ▶ **User Report**
A user report needs to be submitted within 60 days after the Project's finish.

Technical support (optional)

RIST provides technical support for carrying out performance evaluations or detailed analysis of evaluation results as well as optimization of the program for the post-K computer. For receiving this service, you separately submit the application form for technical support.

* The post-K computer will be launched around 2021 as a world-leading, versatile supercomputer, with the goal to develop:
(1) the next generation flagship supercomputer of Japan (the successor of the K)
(2) a wide range of applications that will address social scientific issues of high priority
Website: <https://www.r-ccs.riken.jp/en/postk/project>
** Fujitsu Limited, which is in charge of developing the post-K computer, has cooperated with creation of this environment.

For more details, visit the HPCI portal site (http://www.hpci-office.jp/pages/e_postk_eval_helpdesk) or contact Helpdesk.

| | |
|--------|---|
| E-MAIL | postk-eval-helpdesk@hpci-office.jp |
| URL | http://www.hpci-office.jp/pages/e_postk_eval_helpdesk |

See HPCI Portal site for more details...

* Post-K = Supercomputer **Fugaku**

- **HPCI** was established in 2012 as a national HPC infrastructure
- **Supercomputer Fugaku**, the next flagship system of HPCI and the successor to K computer is scheduled to be operational around 2021.
- **User support** is one of the RIST's roles
- Various kinds of software are already **ready-to-use** for HPCI users now.
- Towards Fugaku, RIST is working for making **OSS ready-to-use** on it, looking ahead to the future collaboration with Arm community.
- Call for project proposals for “**Post-K Computer Performance Evaluation Environment**” is now open, and RIST provides technical supports for them.