

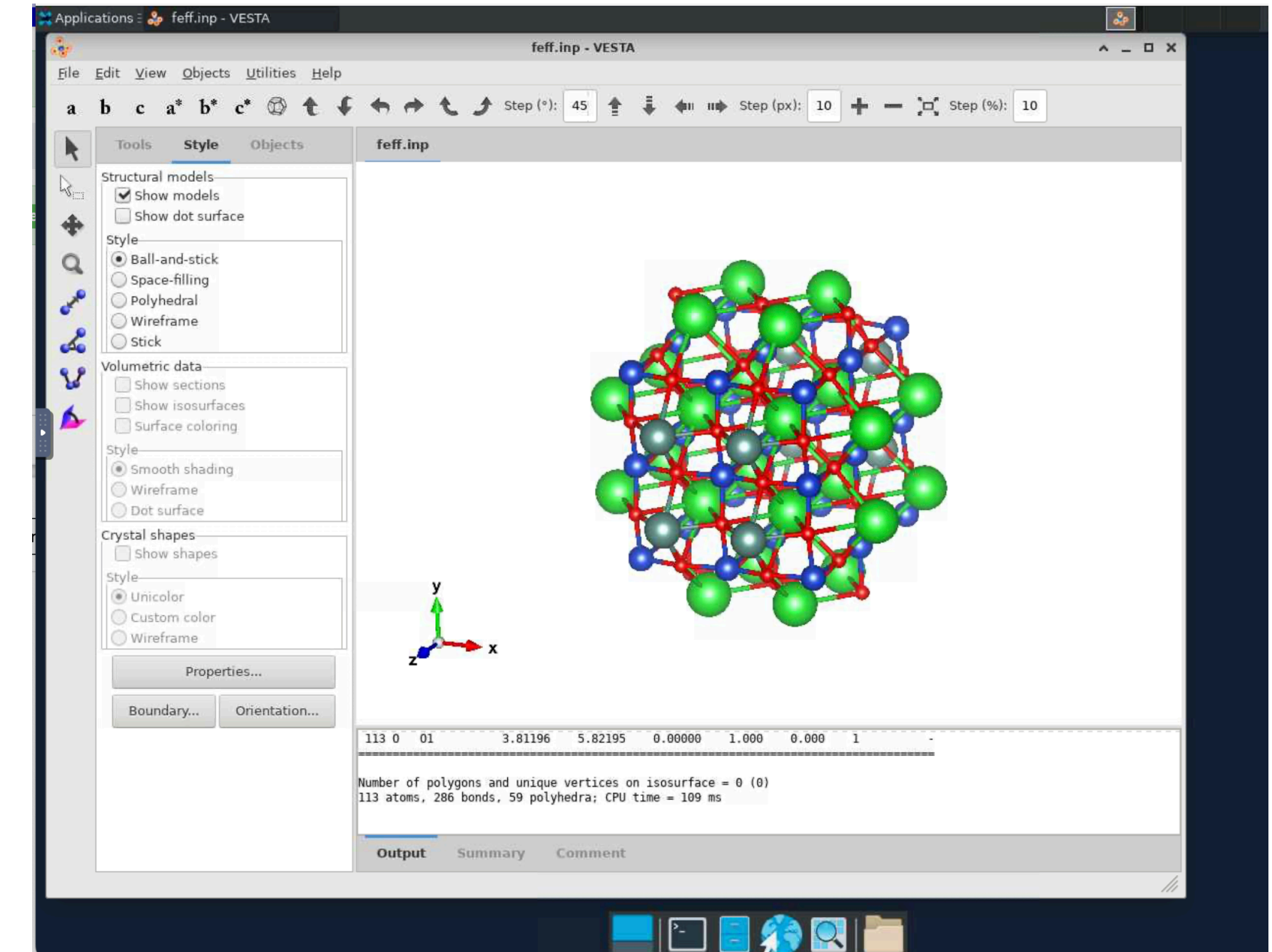


Open OnDemand on Fugaku

Masahiro Nakao (RIKEN R-CCS)

Open OnDemand on Fugaku

- To enhance usability, we have introduced Open OnDemand on Fugaku since 2022
- To fully leverage the capabilities of Open OnDemand, we have implemented the following enhancements[1,2]:
 - Customized the dashboard
 - Implemented interactive applications
 - Developed passenger applications



- [1] Masahiro Nakao, et al. "Introducing Open OnDemand to Supercomputer Fugaku", 10th International Workshop on HPC User Support Tools (HUST2023), Denver, USA, Nov. 2023.
- [2] Masahiro Nakao, Keiji Yamamoto. "Open Composer: A web application for generating and managing batch jobs on HPC clusters", Supercomputing Asia 2025, Singapore, Mar. 2025


Customized the dashboard

- A. Useful external links (e.g., Fugaku manuals)
- B. Failure and operation notices
- C. Number of pending jobs in queues via Grafana
- D. Operation schedule via Google Calendar
- E. Disk and budget usage
- F. Recently used applications (up to 4)
- G. Utilities running on Open OnDemand server
(File upload, job monitoring, and so on)



Significant modifications by customizing the Open OnDemand template

<https://ondemand.fugaku.r-ccs.riken.jp>

Fugaku OnDemandBatch JobsInteractive AppsPassenger AppsMy SessionsDevelopHelpLogged in as a03011Log Out



Welcome to the supercomputer Fugaku

RIKEN Center for Computational Science

Link
OnDemand Manual
Fugaku Portal
Fugaku Schedule
Fugaku Status
Fugaku Support

Message of the day

Information

Jul 24, 2023Operation

July 2023 Large-scale job execution period

Jul 21, 2023Operation

Resource groups during the large scale job execution period

Jul 19, 2023Operation

Occurrence of inaccessibility and poor response at login nodes and jobs due to a file system maintenance(vol0005)

Pending jobs

fugaku-small17867

fugaku-large915

prepost-gpu112

prepost-gpu20

prepost-mem122

prepost-mem23

prepost-ondemand0

Fugaku Schedule

Today1July 2023

Sun	Mon	Tue	Wed	Thu	Fri	Sat
25	26	27	28	29	30	Jul 1
2	3	4	5	6	7	8
9	10	11	12	13	14	15
16	17	18	19	20	21	22
23	24	25	26	27	28	29
30	31	Aug 1	2	3	4	5

Accounting

Updated at 2023/07/25 02:32:10 (JST)

Group	Volume	Disk (GiB)				Disk (inode)				Resource (NH)			
		Limit	Usage	Avail.	Rate	Limit	Usage	Avail.	Rate	Limit	Usage	Avail.	Rate
rccs-aot	/vol0400	5,120	608	4,512	11%	1,500,000	265,259	1,234,741	17%	527,360	81,666	445,693	15%
f-op	/vol0403	614,400	160,260	454,140	26%	180,000,000	144,261,340	35,738,660	80%	-	-	-	-
ra030002	/vol0403	5,120	1	5,119	0%	1,500,000	2	1,499,998	0%	-	-	-	-
/home	/vol0400	20	5	15	25%	200,000	11,619	188,381	5%	-	-	-	-

Recently Used Apps

Desktop

OpenFOAM

SCALE

Jupyter

Passenger Apps

Active Jobs

Home Directory

Gakunin RDM

HPCI Storage

Job Composer

Fugaku Shell Access

A

B

C

D

E

F

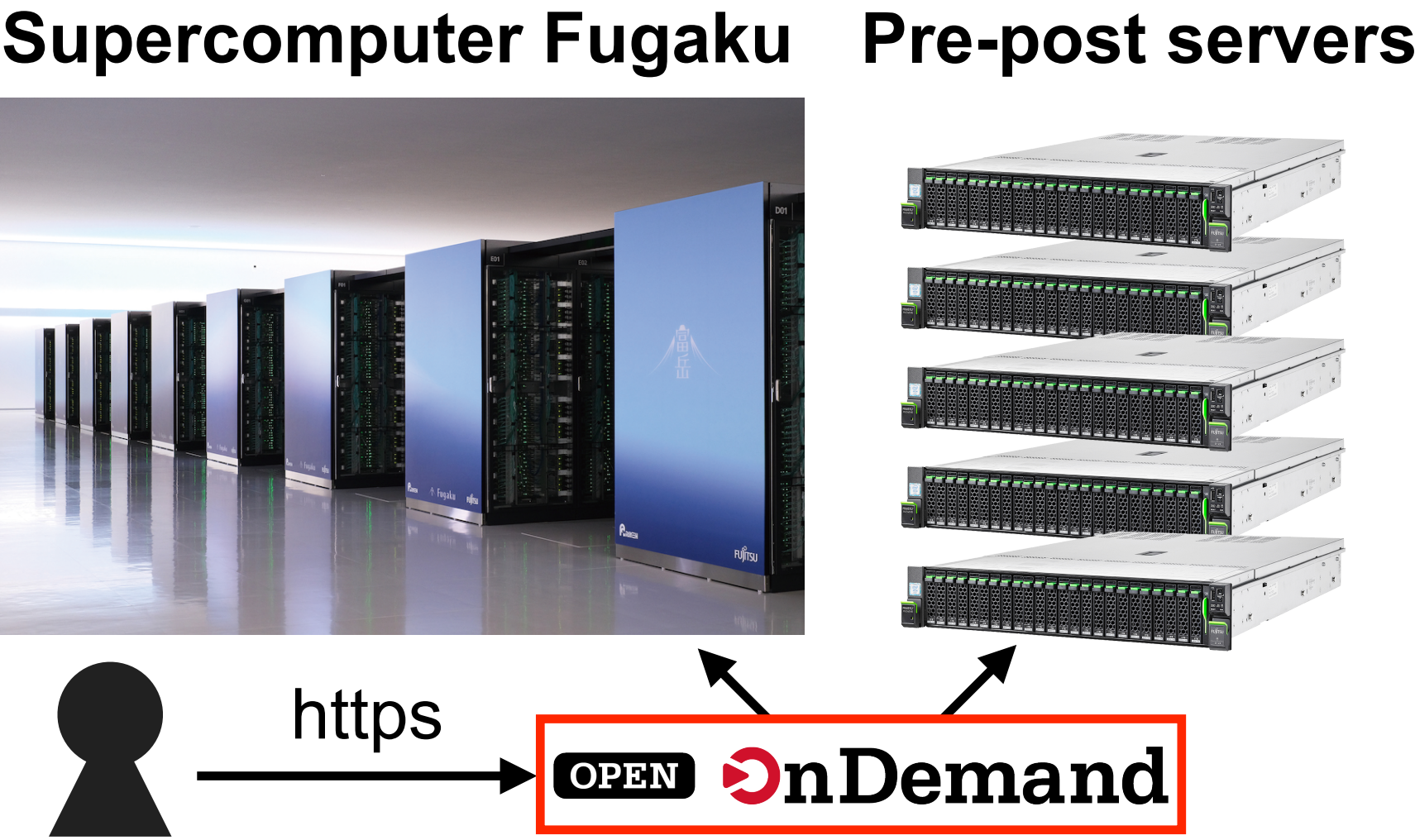
G

3

Implemented interactive applications (1/2)

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

- While **free applications** are installed in singularity container, **commercial applications** are installed locally
- R-CCS provides not only Fugaku but also pre-post servers equipped with Intel CPUs and NVIDIA GPUs
https://github.com/RIKEN-RCCS/ondemand_fugaku.git



Implemented interactive applications (2/2)

Desktop

This app will launch an [Xfce](#) desktop.

System

Fugaku

Resource group

small

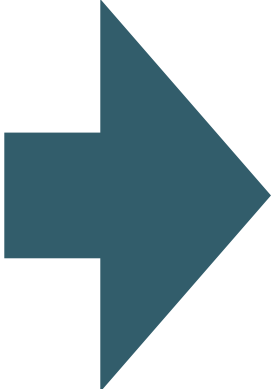
Please refer to the document ([English](#) or [Japanese](#)).

Group

rccs-aot

Maximum run time (1 - 72 hours)

1



Desktop

This app will launch an [Xfce](#) desktop.

System

Prepost

Partition

gpu1

Please refer to the document ([English](#) or [Japanese](#)).

Maximum run time (1 - 3 hours)

1

Number of CPU cores (1 - 72)

1

Number of memory (10 - 186 GB)

10

Number of GPUs (0 - 2)

0

To a submit job to different environments, we use the Dynamic Form Widgets feature in Open OnDemand to dynamically change the options.

Developed passenger applications (1/4)

- Passenger application is a web application that run on Open OnDemand server

- **Disk/Budget Info**

- View your disk usage and budget, as well as those of all group members since these resources are shared across the group

Disk info

Disk usage for each user by group.

rccs-aot (Updated at 2025/05/07 12:47:36 (JST))

User	Volume	Path	Capacity [GiB]				Inode			
			Limit	Usage	Avail.	Ratio	Limit	Usage	Avail.	Ratio
a03002	/vol0400	/data/rccs-aot, /share/rccs-aot	5,120	5	3,969	0.09%	1,500,000	42	446,080	0.0%
a03003	/vol0400	/data/rccs-aot, /share/rccs-aot	5,120	456	3,969	3.9%	1,500,000	10,421	446,080	0.69%
a03011	/vol0001	/2ndfs/rccs-aot	5,120	64	3,969	1.25%	1,500,000	3,399	446,080	0.22%

Budget info (Updated at 2025/05/07 05:01:40 (JST))

Budget usage for each user by group.

rccs-aot

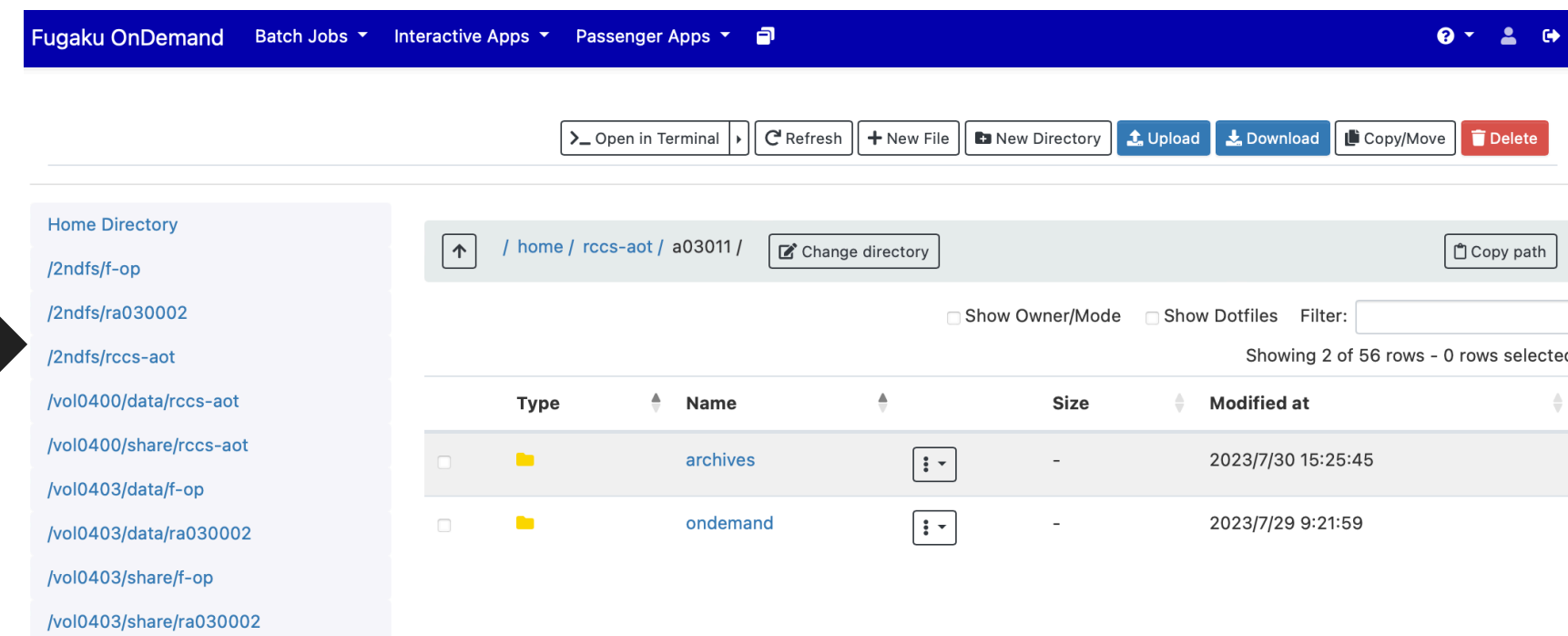
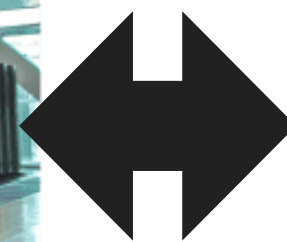
User	Budget [NH]				
	Limit	Usage	Available	Ratio	Change Limit (For only a theme manager)
a03011	227,360	14	196,933	0.0%	227360 submit
a03012	227,360	27	196,933	0.01%	227360 submit
(Exclusive Use)	227,360	30,384	196,933	13.36%	227360 submit

Developed passenger applications (2/4)

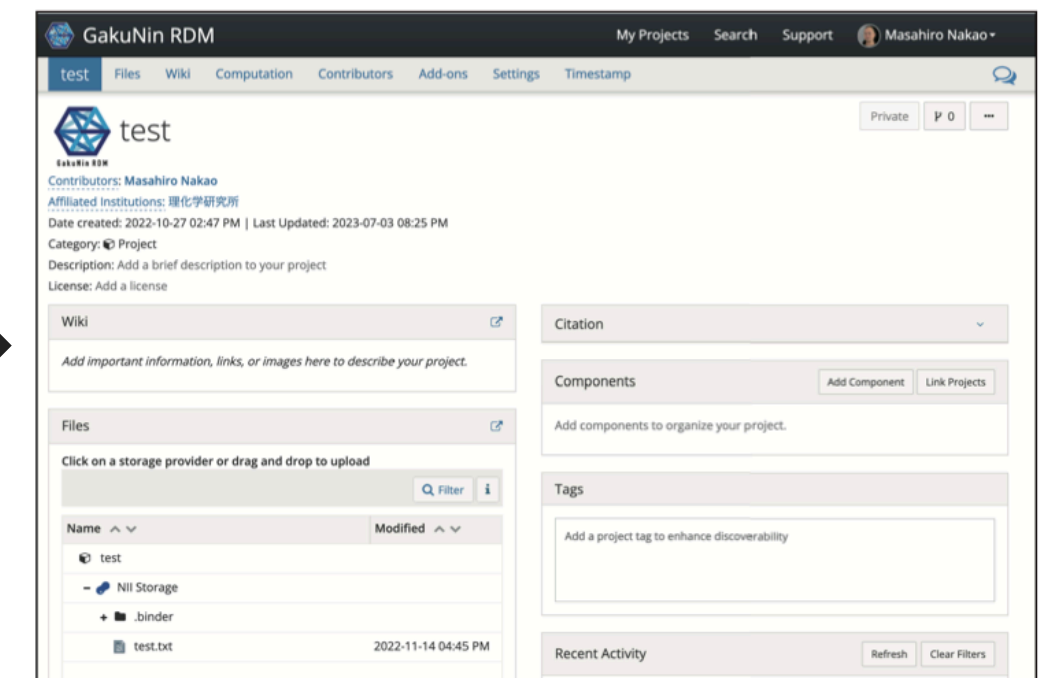
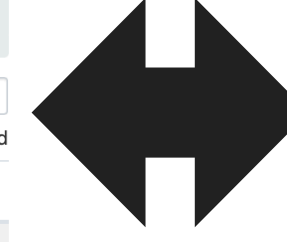
- HPCI Shared Storage/GakuNin RDM Access
 - These are external storages in Japan for research
 - These applications perform mounting the storages
 - File operations can be performed using the Home Directory of Open OnDemand after mounting the storages



HPCI Shared Storage



Home Directory of Open OnDemand



GakuNin RDM

Developed passenger applications (3/4)

- **Open Composer** <https://github.com/RIKEN-RCCS/OpenComposer>
 - Open source software, support Slurm, PBS, GridEngine, Fujitsu TCS
 - Submit and manage a batch job
 - When you enter items on the left page, a job script is generated on the right page
 - The job script is editable
 - Click the "Submit" button to register the generated job script in the job scheduler
 - See DEMO

The screenshot displays the Open Composer web interface. At the top, there are navigation links: "Top", "Application" (with a dropdown arrow), and "History". On the far right of the top bar is a link "Open OnDemand". The main content area is divided into two columns. The left column has a purple header with the text "test" and "This is test." below it. Below this, there are configuration options: "Queue" with radio buttons for "small" (selected) and "large"; "Max hours (0-24)" with a dropdown set to "1"; "Max minutes (0-59)" with a dropdown set to "0"; "Number of nodes (1 - 128)" with a dropdown set to "4"; and "Executable binary" with a text input field containing "/Users/mnakao/" and a "Select Path" button. The right column has a purple header with "Script Location*" and a text input field containing "/Users/mnakao/" with a "Select Path" button. Below this is "Script Name*" with a text input field containing "job.sh" and "Job Name" with an empty text input field. Further down is "Script Contents" with a large text area containing the following script:

```
#!/bin/bash
#PJM -L "rscgrp=small"
#PJM-L "elapsed=1:0:00"
#PJM-L "node=4"
mpiexec /Users/mnakao/
```

 At the bottom of the right column is a large blue "Submit" button. The footer of the interface shows "Open Composer version: 1.0.0".

Developed passenger applications (4/4)

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

There are 25 applications available on Fugaku Open Composer. These applications are configured in consultation with the developers and users of each application.

Summary

- We have introduced Open OnDemand on Fugaku with the following customizations
 - Customized the dashboard
 - Implemented interactive applications
 - Developed passenger applications
- Open OnDemand usage status on Fugaku
 - The number of Open OnDemand users has been increasing
 - The number of Fugaku users at the end of 2024 was 4,900, so 25% of the users have experience using Fugaku Open OnDemand

