



Building the Open OnDemand Community at RIKEN R-CCS

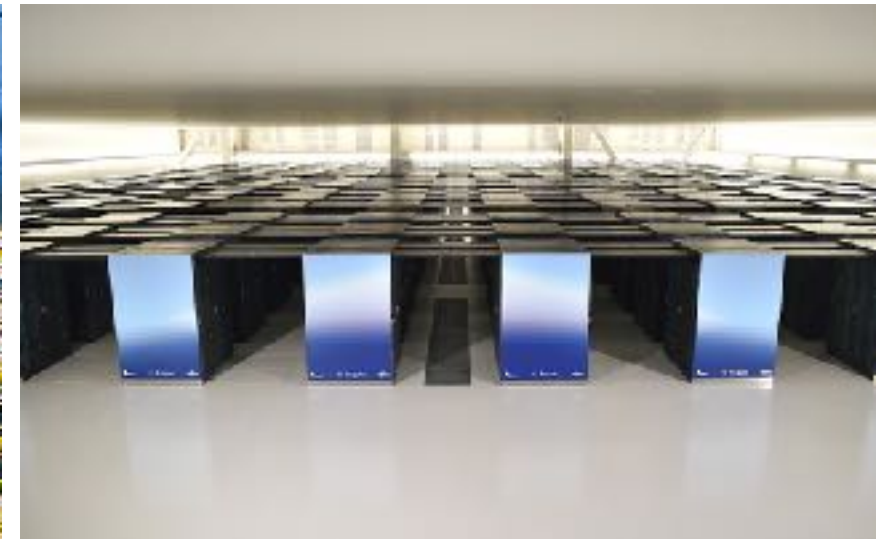
Masahiro Nakao (RIKEN R-CCS)



Partner Talk at Open OnDemand Booth

Supercomputer Fugaku

- We have been operating the supercomputer Fugaku, a Japanese flagship super-computer, since 2021
- Located in RIKEN Center for Computational Science in Kobe city, Japan
- About 160,000 compute nodes
- Graph500, HPCG: 1st, HPL-AI: 3rd, Top500: 4th



Open OnDemand in Japan

- We had run test operations of Open OnDemand on Fugaku since Aug. 2022, and have run production operations since May 2023
- Open OnDemand is also attracting attention at other national research institutes and supercomputer centers in Japan
- To spread our experience, we held some events in Japan
 - Programming contest for high school students [1]
 - Open OnDemand Workshop in PC Cluster Consortium [2]
 - Meeting for application code tuning on A64FX computer systems [3]
 - Other application courses, etc.

[1] <https://www.gsic.titech.ac.jp/supercon/main/attwiki/index.php>

[2] <https://www.pccluster.org/ja/event/2023/09/231011-ws-openondemand.html>

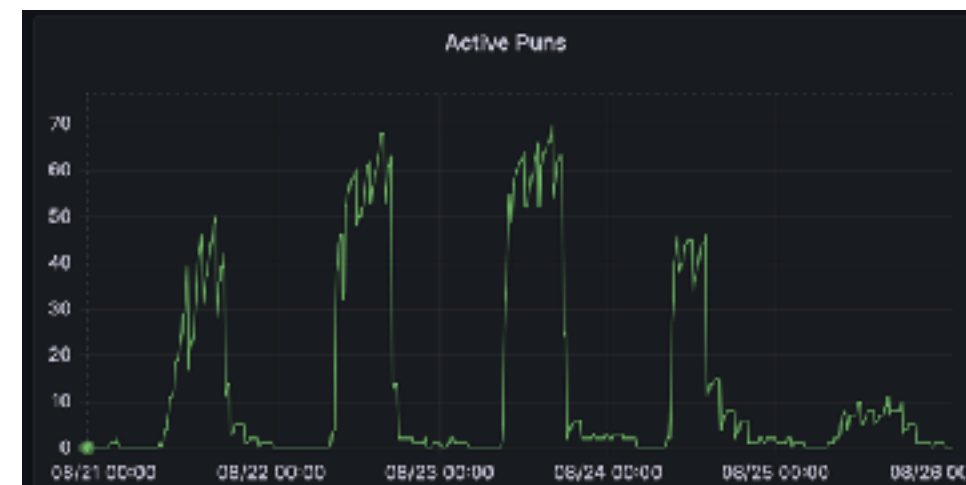
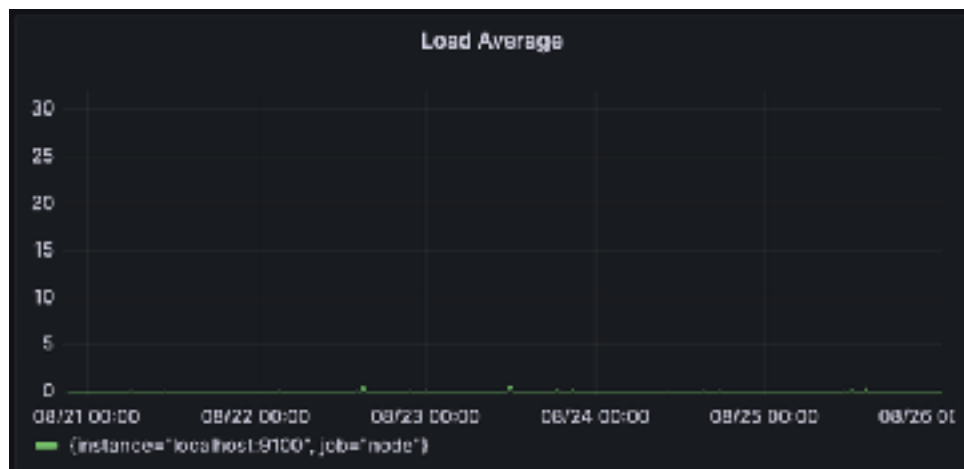
[3] https://www.hpci-office.jp/en/events/symposia/meeting_A64FX_231023



Supercomputing contest on Fugaku

- A supercon for high school students was held from August 21st to 25th, 2023
- Fugaku was be used from 2021
- This year we use Open OnDemand instead of SSH
- There is no longer an explanation about using PuTTY and WinSCP, and how to generate and register SSH keys
- The description is OS independent

Open OnDemand
has a very low load



Open OnDemand on Fugaku

- This presentation describes how we introduced Open OnDemand to Fugaku
 - Display of useful information for users on the dashboard
 - Support for Fujitsu TCS, Fugaku job scheduler
 - About 50 applications are now available from Open OnDemand
 - Develop applications to connect with external storages
- The configuration files can be downloaded from https://github.com/RIKEN-RCCS/ondemand_fugaku

Open OnDemand

Welcome to the supercomputer Fugaku

Message of the day

Information

- Jul 04, 2023 Operation: July 2023 Large-scale job execution period
- Jul 21, 2023 Operation: Resource group (during the large-scale job execution)
- Jul 10, 2023 Operation: Occurrence of inaccessibility and poor response at login nodes and jobs due to a file system node resource (RCCS)

Pending jobs

Job ID	Resource Group	Queue	Job Name	Status
fugaku-1001	1001	1001	1001	1001
fugaku-1002	1002	1002	1002	1002
fugaku-1003	1003	1003	1003	1003
fugaku-1004	1004	1004	1004	1004
fugaku-1005	1005	1005	1005	1005
fugaku-1006	1006	1006	1006	1006
fugaku-1007	1007	1007	1007	1007
fugaku-1008	1008	1008	1008	1008
fugaku-1009	1009	1009	1009	1009
fugaku-1010	1010	1010	1010	1010

Accounting

Group	Volume	Unit	Usage	Limit	Usage	Limit	Usage	Limit	Usage	Limit	Usage	Limit
user	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000
group	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000
project	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000
system	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000

Recently Used Apps

- Desktop
- Open OnDemand
- SCCCE
- Open OnDemand

Peripheral Apps

- Active Job
- Home Directory
- Submit B2B
- HPC Storage
- Job Composer
- Fugaku Shell access

Dashboard of Open OnDemand on Fugaku

- A. External links (Fugaku manual, etc.)
- B. Failure information, operation information, etc.
- C. Number of waiting jobs in each queue using Grafana
- D. Operational calendar using Google Calendar
- E. User disk and budget utilization
- F. Apps that run on recently used compute nodes
 - Interactive application (GUI jobs and Batch Jobs)
 - Other apps can be selected from a navigation bar
- G. Utilities that work with Open OnDemand server
 - Passenger application
 - File upload, job monitoring, etc.

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

The screenshot displays the Open OnDemand dashboard for Fugaku. The interface includes a top navigation bar with links for documentation, batch jobs, interactive jobs, storage, and sessions. The main content area is divided into several sections:

- Welcome to the supercomputer Fugaku**: A header section with the RIKEN logo and a message of the day.
- Information**: A section providing operational status and messages, such as "July 24, 2023: Operation: July 2023 large-scale job execution period".
- Pending Jobs**: A section showing the number of pending jobs in different queues, represented by colored bars (red for 'fugaku-std', green for 'fugaku-std-1', etc.).
- Accounting**: A table showing resource usage and accounting information for various users and groups.
- Recently Used Apps**: A section displaying icons for applications like Docker, Open OnDemand, and others.
- Passenger Apps**: A section displaying icons for applications like ActiveJobs, Home Directory, and others.

Labels A through G are placed next to specific sections of the dashboard to indicate their corresponding items in the list:

- A: External links (Fugaku manual, etc.)
- B: Failure information, operation information, etc.
- C: Number of waiting jobs in each queue using Grafana
- D: Operational calendar using Google Calendar
- E: User disk and budget utilization
- F: Apps that run on recently used compute nodes
- G: Utilities that work with Open OnDemand server

Dashboard of Open OnDemand on Fugaku

```
<%-
  require 'utils.rb'
  info = dashboard_info("/system/ood/motd/info.txt")
-%>

:
<h4>Information</h4>
<table>
<%- info.each do |i| -%>
  <tr>
    <%- c = i.split(":") -%>
    <td><%= c[0] %></td><td><%= c[1] %></td><td><%= c[2] %></td>
  </tr>
<%- end -%>
</table>
```

B

Information

Jul 24, 2023

Operation

July 2023 Large-scale job execution period

Jul 21, 2023

Operation

Resource groups during the large scale job execution period

Jul 19, 2023

Operation

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

The info.txt is updated once a day by cron.
The info.txt is generated from the information on the Fugaku portal site.
Disk usage and budget information are the same.

E

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
roce-301	/vol0400	5,120	608	4,512	11%	1,500,000	265,259	1,234,741	17%	527,360	81,888	445,663	16%
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%	-	-	-	-

Dashboard of Open OnDemand on Fugaku

```
<%-
require 'time'

# URL of Dashboard
dashboard_url = "https://status.fugaku.r-ccs.riken.jp/d-solo/cf06d886-
e672-41d8-a587-85ccb32fce7e/
5a6f6KGM5b6F44Gh44K444On44OW5pWw?
orgId=1&theme=light&panelId=2"

# Get the current time as epoch milliseconds.
now = (Time.now.to_f * 1000).to_i

# Get time one month ago as epoch milliseconds
one_month_ago = now - (30 * 24 * 60 * 60 * 1000)
-%>

:
<h4>Pending Jobs</h4>
<iframe src="<%= dashboard_url %>&to=<%= now %>&from=<%=
one_month_ago %>" frameborder="0" width="100%" height="225px">
</iframe>
```

Grafana and Google Calendar have the abilities to port graphs to external HTML.



Development of adapter for Fujitsu TCS

- Open OnDemand supports various job schedulers
 - Slurm, Torque, PBS, and so on
 - Fujitsu TCS did not be supported
- Open OnDemand provides an adapter interface to support various job schedulers

submit Submit a job
delete Delete a job
status Get status of a job
hold Hold a job
release Release a held job
info Get information for a job
info_all Get information for all jobs
cluster_info Get system information for an HPC cluster
supports_job_arrays Bulk job support availability

We developed an adapter for Fujitsu TCS by implementing these methods defined in the parent class in Ruby language (about 400 lines).

This addition has been merged into the Open OnDemand GitHub repository, so Open OnDemand is now available for Fujitsu TCS.

Add applications

- In Fugaku, applications are managed by spack
 - Set the environment variables using **spack load** command from Open OnDemand
- Some interactive applications (Remote desktop etc.) are not installed on Fugaku
 - Create a container image using Singularity
 - Run the applications using **singularity run** command from Open OnDemand

Applications

● Interactive Application

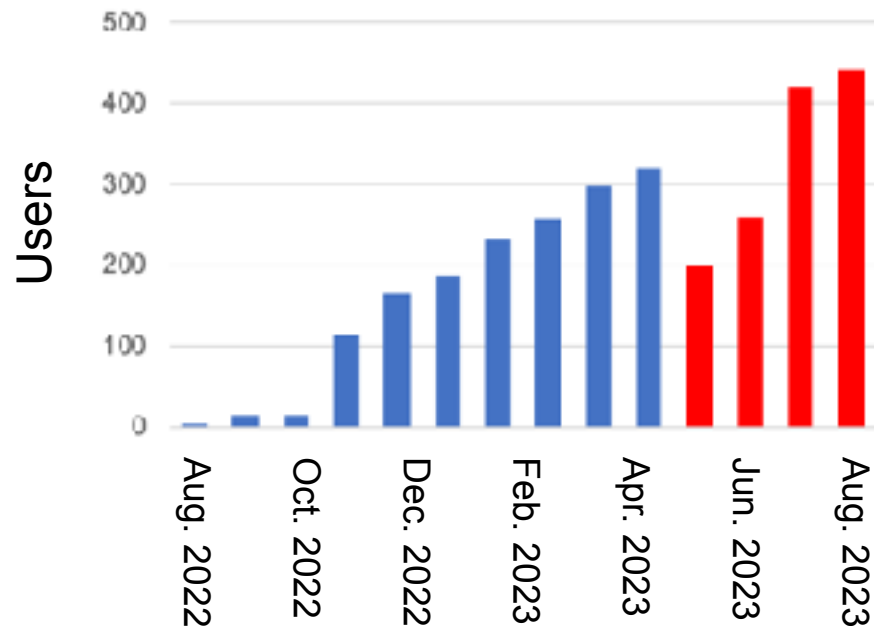
Category	Application
Development	Remote Desktop , JupyterLab , MATLAB, RStudio , VSCode
Profiler	NVIDIA Visual Profiler, NVIDIA Nsight Compute*, NVIDIA Nsight Systems, Vampir
Viewer	AVS/Express, C-Tools , GaussView, ImageJ , OVITO , Paraview , PyMOL , SALMON view, Smokeview , VESTA , VMD , VisIt , XCrySDen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

● Batch Job (Not operated interactively)

Managed by singularity

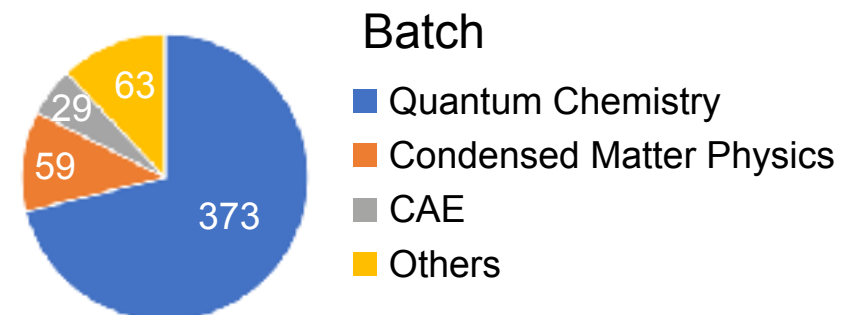
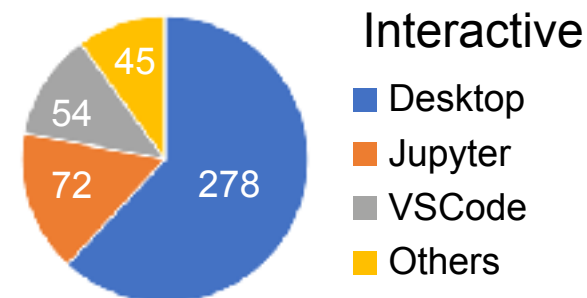
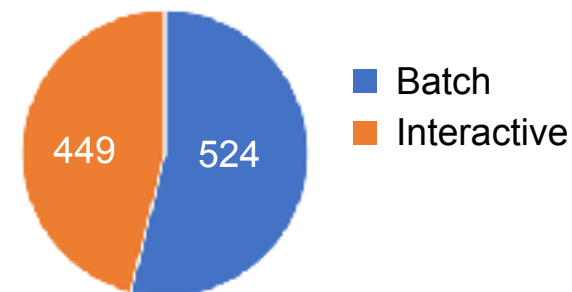
Category	Application
Climate	SCALE
Computer Aided Engineering	FDS, FrontFlow (blue/X), FrontISTR, OpenFOAM (Foundation/OpenCFD)
Condensed Matter Physics	ALAMODE, AkaiKKR, H Φ , mVMC, OpenMX, PHASE/0, Quantum Espresso, SALMON
Molecular Dynamics	GENESIS, GROMACS, LAMMPS, MODYLAS
Quantum Chemistry	ABINIT-MP,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

Status on Fugaku



Since we switched to a new server in May 2023, we have been re-counting the number of new users. The number of users as of today (15th Nov. 2023) is **548**. The number of Fugaku accounts is about 2,500. The graph above is a cumulative number, so it also includes deleted users.

Job type from May to Aug. 2023

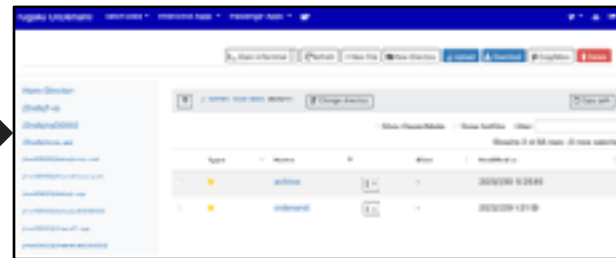
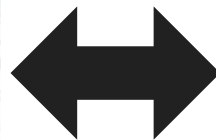


Transferring data to external storage

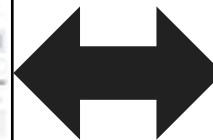
- Applications on Open OnDemand for **HPCI Shared Storage** and **GakuNin RDM**
 - **HPCI Shared Storage** is a large-scale data sharing infrastructure for high-speed of research data among Japanese research organizations
 - **GakuNin RDM** is a research data management service for sharing research data with collaborators
- Users can share data between Open OnDemand and these storages in your web browser by a high-speed network called **SINET6**



HPCI Shared Storage



Open OnDemand on Fugaku



GakuNin RDM



The rclone does not support these storages.

Transferring data to external storage

- Developed using the framework provided by Open OnDemand
- <https://osc.github.io/ood-documentation/latest/tutorials/tutorials-passenger-apps.html>



The screenshot shows the Fugaku Open OnDemand interface. At the top, there's a navigation bar with links like 'Home', 'About', 'Help', and 'Logout'. Below the navigation bar, there's a 'Welcome to the supercomputer Fugaku' message. The main content area is divided into several sections: 'Message of the day', 'Information', 'Pending jobs', 'Accounting', 'Recently Used Apps', and 'Passenger Apps'. The 'Passenger Apps' section is highlighted with a red box, and a red arrow points to it with the word 'Click' in a red box.

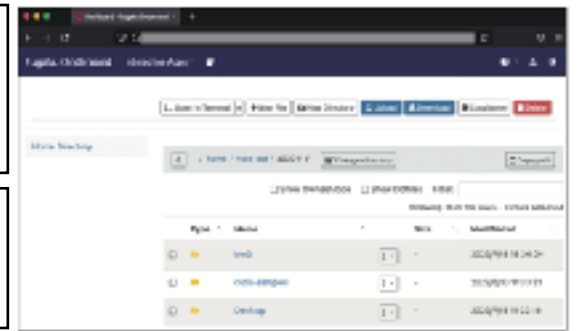
HPCI Storage

Please issue a proxy certificate with the HPCI Certificate Issuing System before mounting the HPCI storage.

Action	HPCI ID	Elapsed time (up to 168 hours)	Passphrase	Mount Path
mount	<input type="text"/>	12 <input type="text"/>	<input type="text"/>	<input type="text"/>

GakuNin RDM

Available Actions	MOUNT_PATH	RDM_NODE_ID	RDM_TOKEN
mount	<input type="text"/>	<input type="text"/>	<input type="text"/>

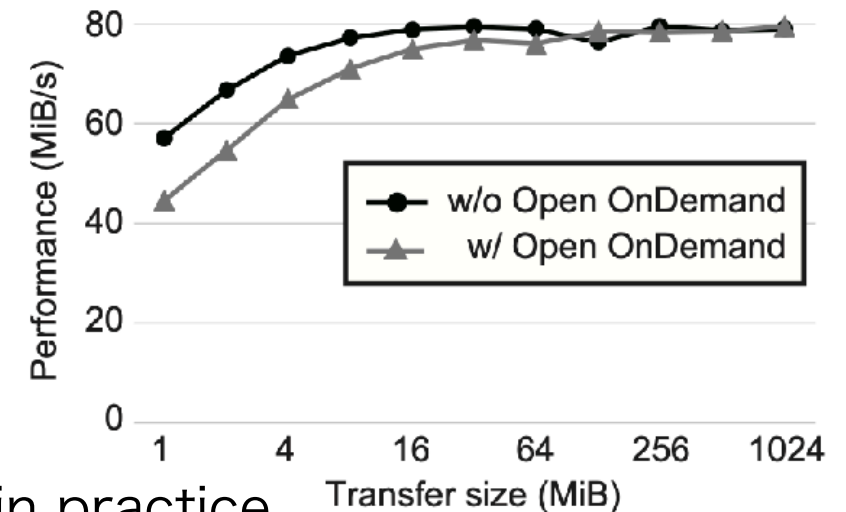


The screenshot shows the 'Home' directory application interface. It features a navigation bar with links like 'Home', 'About', 'Help', and 'Logout'. Below the navigation bar, there's a 'Welcome to the supercomputer Fugaku' message. The main content area displays a list of files and directories, including 'home', 'root', and 'tmp'. A red box highlights the 'home' directory, and a red arrow points to it with the word 'Click' in a red box.

- After inputting the required information, mount on each storage
- Launch the home directory application to upload files to each storage

Transferring data to external storage

- Evaluate transfer speed
 - To examine the overhead of Open OnDemand, compare data transfer speeds with and without Open OnDemand
 - Transfer data from Open OnDemand web server to HPCI shared storage
 - Open OnDemand web server and HPCI shared storage are in the same building
 - Open OnDemand web server CPU: Xeon Gold 6338 x2, Memory: 256GB, network: 100Gbps
- Result
 - Up to 28% faster without Open OnDemand
 - As the data size increases, the performance difference decreases. There is no difference in performance above 64MiB, so there is no problem in practice



Summary

- Introduce the spread of Open OnDemand in Japan
- Hold some Open OnDemand events
- Install Open OnDemand on Fugaku
 - Development an adapter for Fujitsu TCS
 - Display of useful information for users on the dashboard
 - Install about 50 applications
 - Development of data transfer application for external storages