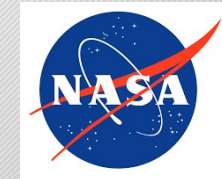


Open On Demand

About Me: Greg Gutmann

Past

- NASA Goddard Space Flight Center (2013-2015)
- Tokyo Institute of Technology: PhD (2016)
- Tokyo Institute of Technology: Assistant Professor (2017-2022)



Present

- Nvidia Deep Learning Institute Instructor (2018-)
- Molecular Robotics Research Institute (2020-)
- Computational Science K.K. (2022-)



DEEP
LEARNING
INSTITUTE



分子ロボット総合研究所
生体分子で創る人工物の世界

Focus

- HPC: GPGPU Specialization
- Networking: TCP/UDP
- Visualization: Real-time simulation, VR
- Robotics: Drone, 3D Printing



Open OnDemand: Introduction

HPC Access

- Historically HPC has relied on command-line interfaces
- Ohio Supercomputer Center (OSC) has developed **Open OnDemand** a graphical interface for HPC
- **Open OnDemand** is:
 - A web interface to interface with HPC resources
 - Enables more users to benefit from HPC
 - Simplifies aspects of HPC for advanced users too



Open OnDemand's History

2013 - OnDemand Reveal

2015 - National Science Foundation (NSF) Funding to make Open OnDemand

2019 - 50 Known users

2021 - Google grant to use OnDemand on Google Cloud

2022 - 250 Known installations

2027 - NSF funding is up for renewal



<https://openondemand.org/read-our-story>

HPC Modeling and Simulation

For Commercial Customers

- Computer-aided design and Engineering (CAD/CAE) simulation on local machines is often limited
- OSC & AweSim collaborated to provide:
 - Modeling and simulation M&S-as-a-service
 - RF, Thermodynamics, Aerodynamics, Electromagnetic, Mechanical
- TotalSim US one of the largest OSC OnDemand users
 - Focused on CFD simulation

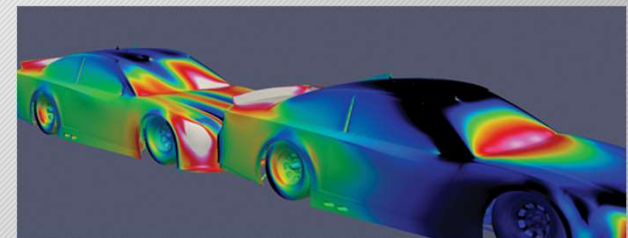


Industry Usage of OnDemand

- NASCAR: CFD simulations for car body design
 - OnDemand: Reduced cost by an order of magnitude (~35k to ~3k USD)
 - OnDemand: Enabled running 5x more simulations

Benefits of OnDemand HPC

- **Offers a more efficient interface**
- Handle burst of high demand usage
- Reduces idle time of HPC resources
- Can be maintained by IT specialists



HPC Wire: NASCAR race car CFD simulation running on OSC Owens supercomputer

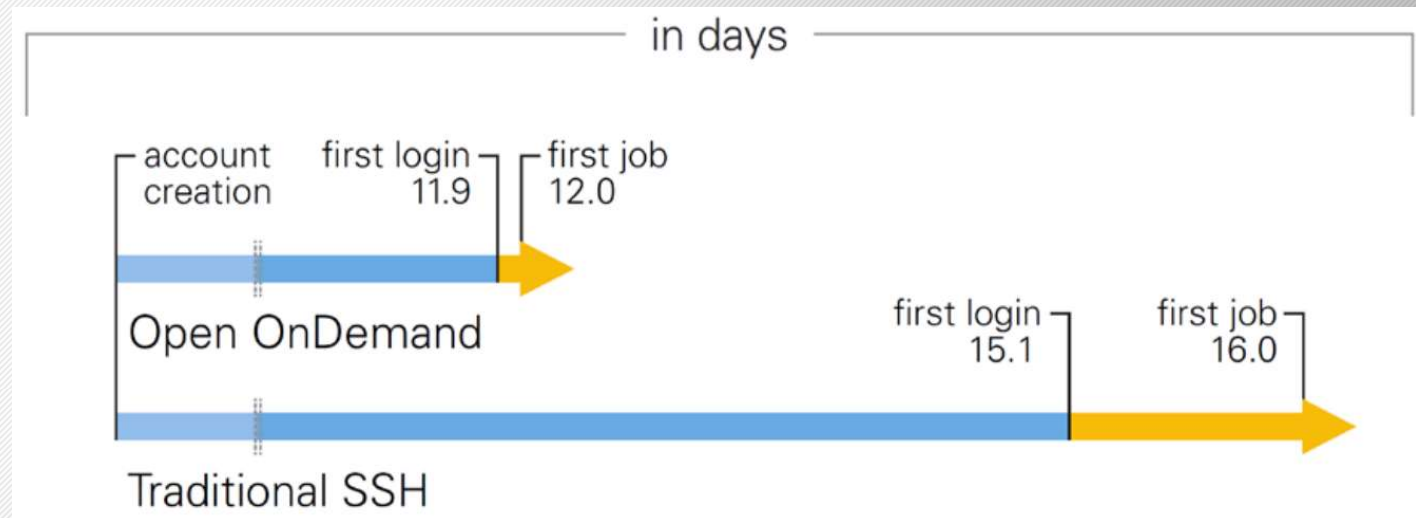
OnDemand User Study

from The Ohio Supercomputer Center

OnDemand users start work faster than traditional users

In terms of:

- First login
- Job submission



Impact at The Ohio Supercomputer Center*

* <https://www.nitrd.gov/nitrdgroups/images/c/cb/MAGIC-2019-06-Alan-Chalker.pdf>

OnDemand User Study

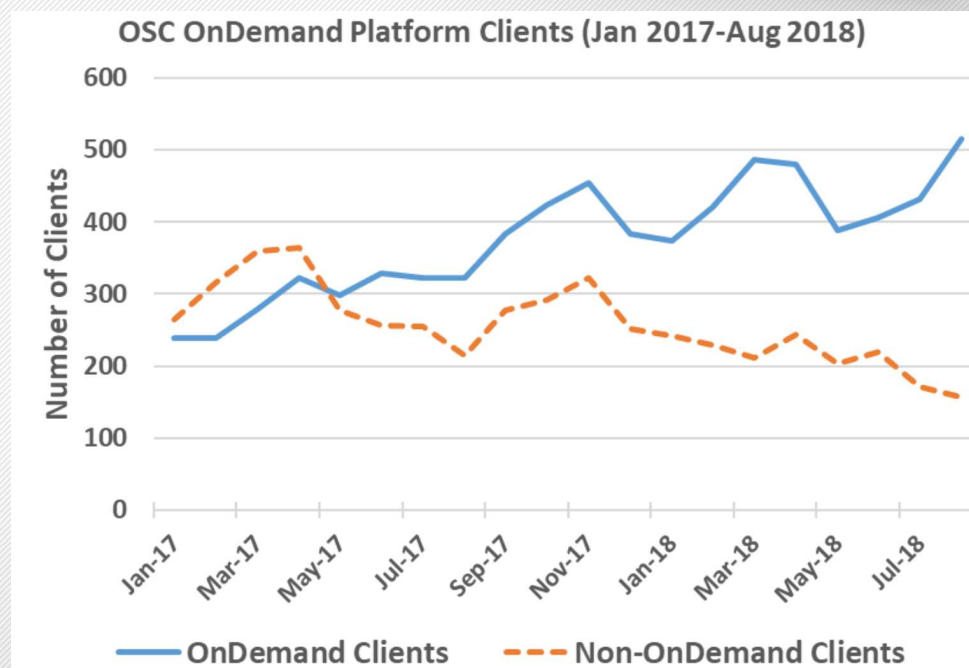
from The Ohio Supercomputer Center

- OSC saw a steady migration from:

Non-OnDemand clients



OnDemand clients



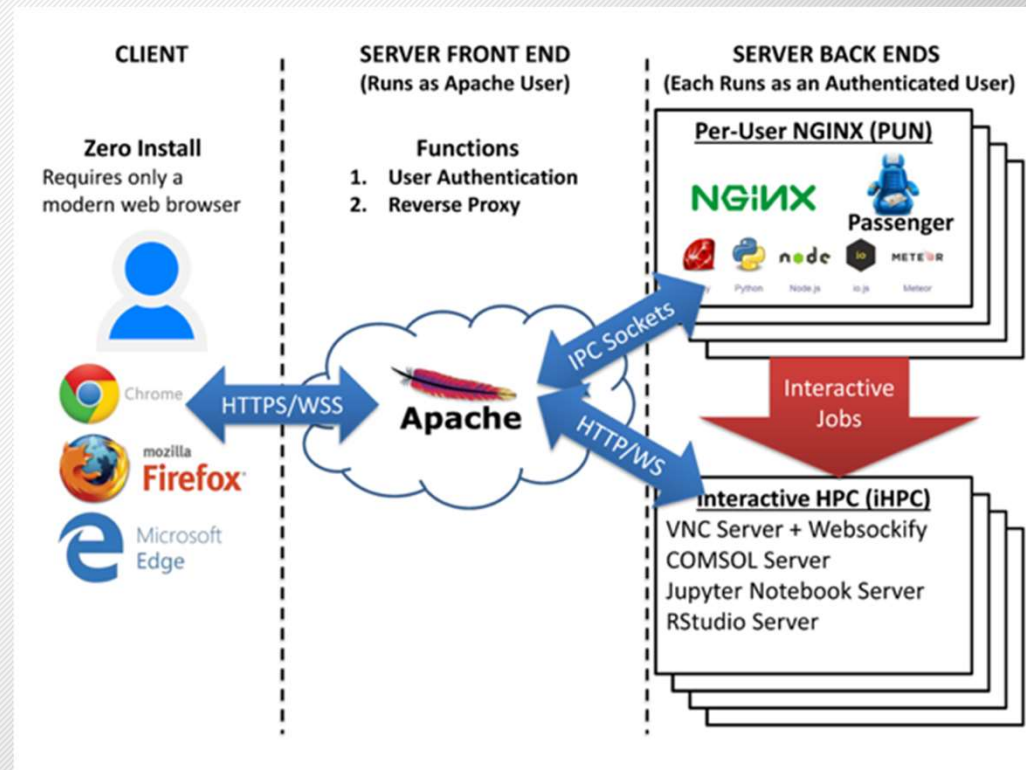
Impact at The Ohio Supercomputer Center*

* <https://www.nitrd.gov/nitrdgroups/images/c/cb/MAGIC-2019-06-Alan-Chalker.pdf>

Architecture & Security

Architecture Overview

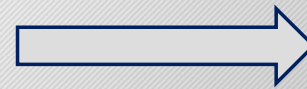
- Zero Install for User
- Secure Server Front End
- Backend
 - Customizable
 - Scalable



<https://osc.github.io/ood-documentation/latest/architecture.html>

Security measures

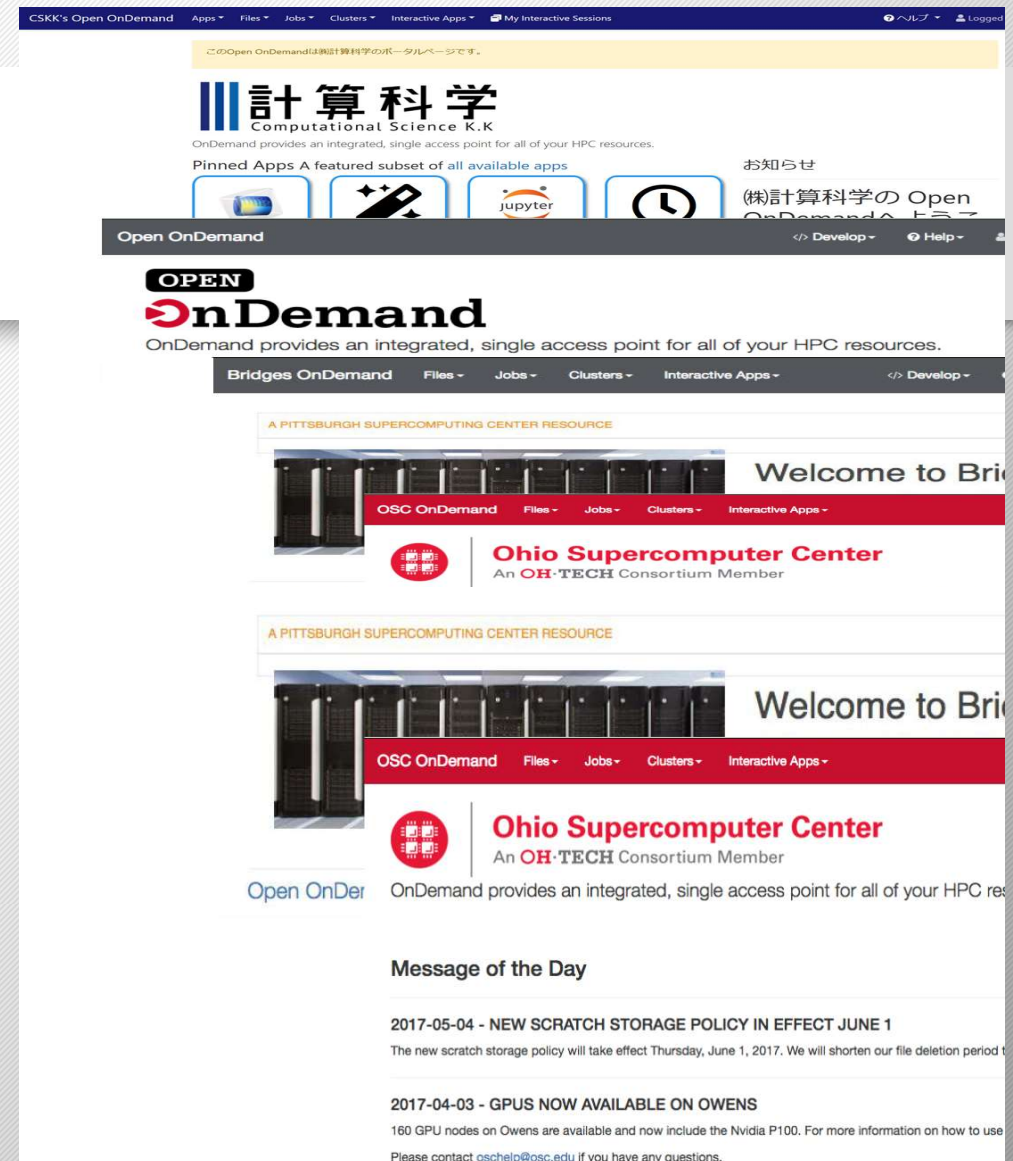
- HTTPS / SSL ---- *Encrypted connections*
- Firewall ----- *Network traffic control*
- LDAP ----- *Secure resource access*
- Reverse Proxy -- *Eliminates direct communication to server*
- Login authentication with OpenID
 - Third-party identity provider (IDP) service
 - Eliminating the need for webmasters to provide their own ad hoc login systems



On Demand Features

Custom Branding

- Navbar Configurations: Nearly every aspect of the navbar can be customized.
- Profiles: to significantly alter the appearance.
- Custom Landing Pages with dedicated URLs



<https://www.nitrd.gov/nitrdgroups/images/c/cb/MAGIC-2019-06-Alan-Chalker.pdf>
https://www.osc.edu/press/open_ondemand_30_makes_hpc_even_easier_with_advanced_community_driven_upgrades

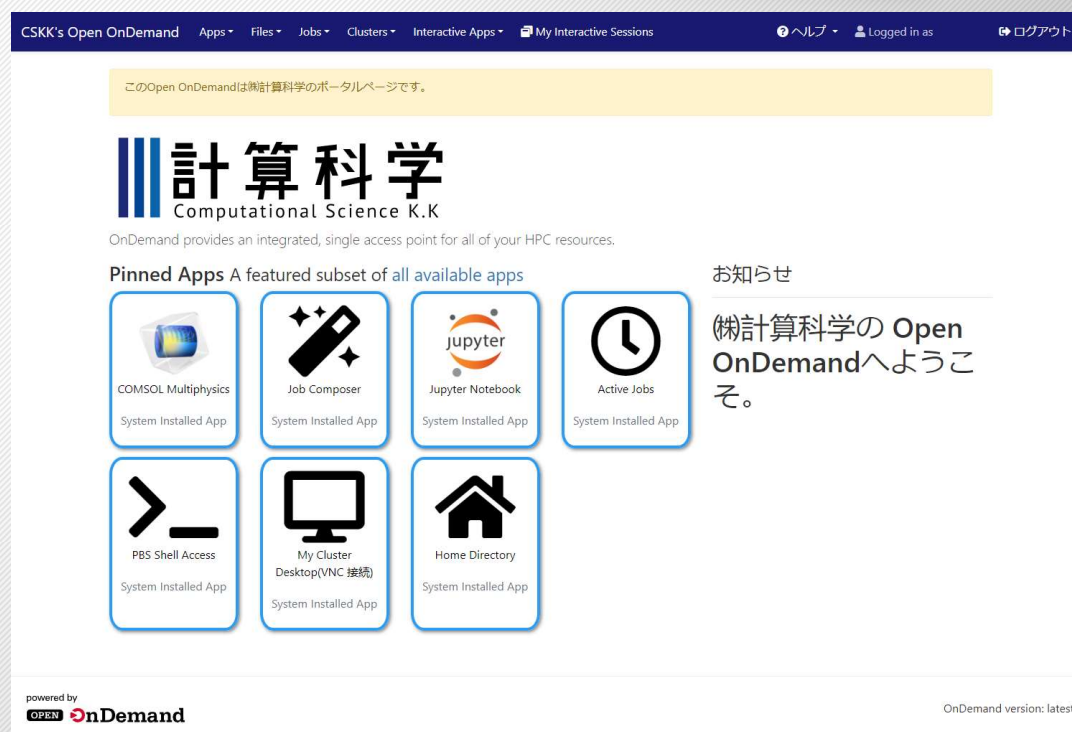
Supported Features Overview

Applications

- Abaqus
- ANSYS
- COMSOL
- MATLAB
- Jupyter
- RStudio
- QGIS
- Paraview
- STATA
- Tensorboard

Job schedulers

- PBS Pro
- SLURM
- Grid Engine
- Torque
- LSF

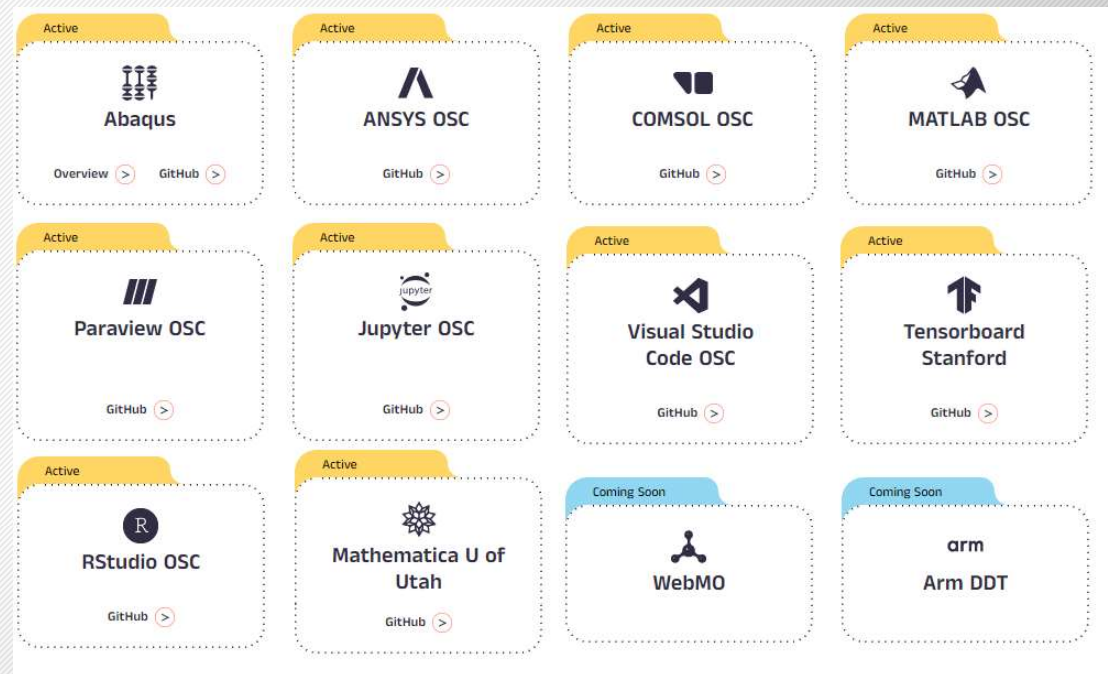


https://www.cskk.jp/product_solution/open-ondemand

Application Support Projects

Available on GitHub/GitLab

- Active community
- Support for new applications over time
- Application support can be added by users or by supporting groups such as CSKK



More applications can be found here:
<https://openondemand.org/run-open-ondemand>

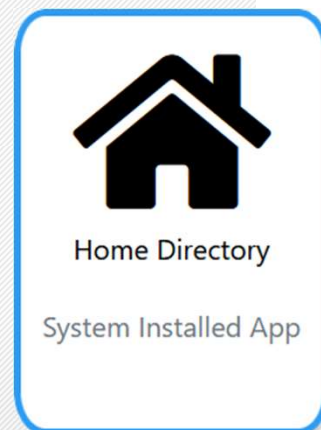
Live Demonstration

Offline Demonstration

Home Directory

OnDemand allows users to:

- View
- Edit
- Upload
- Download files



CSKK's Open OnDemand Apps Files Jobs Clusters Interactive Apps

このOpen OnDemandは計算科学のポータルページです。

Open in Terminal Refresh New File New Directory Upload Download Copy/Move Delete

Home Directory

↑ / nfs / home / gutmann / Drone / Change directory Copy path

☐ Show Owner/Mode ☐ Show Dotfiles Filter:

Showing 13 of 14 rows - 0 rows selected

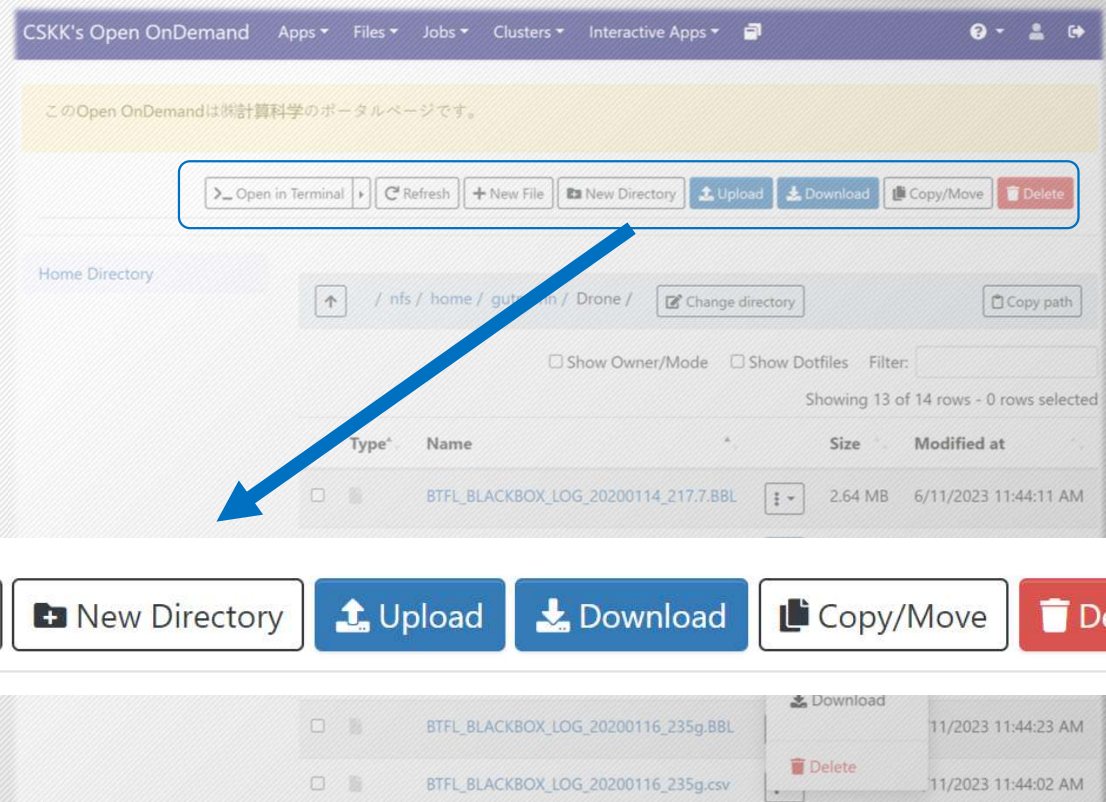
Type	Name	Size	Modified at
<input type="checkbox"/>	BTFL_BLACKBOX_LOG_20200114_217.7.BBL	2.64 MB	6/11/2023 11:44:11 AM
<input type="checkbox"/>	BTFL_BLACKBOX_LOG_20200114_217.7.csv	21.3 MB	6/11/2023 11:44:15 AM
<input type="checkbox"/>	BTFL_BLACKBOX_LOG_20200115_200g.BBL		11/2023 11:44:16 AM
<input type="checkbox"/>	BTFL_BLACKBOX_LOG_20200115_200g.csv		11/2023 11:44:22 AM
<input type="checkbox"/>	BTFL_BLACKBOX_LOG_20200116_235g.BBL		11/2023 11:44:23 AM
<input type="checkbox"/>	BTFL_BLACKBOX_LOG_20200116_235g.csv		11/2023 11:44:02 AM

View Edit Rename Download Delete

Home Directory

OnDemand allows users to:

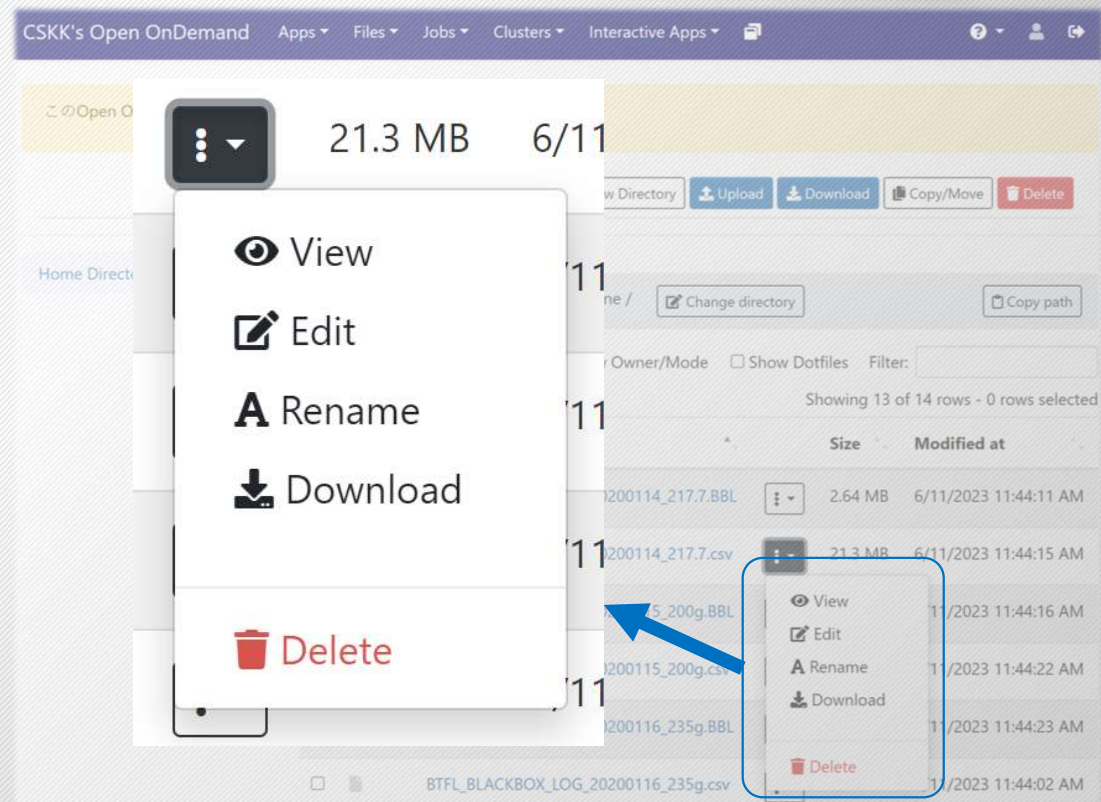
- View
- Edit
- Upload
- Download files



Home Directory

OnDemand allows users to:

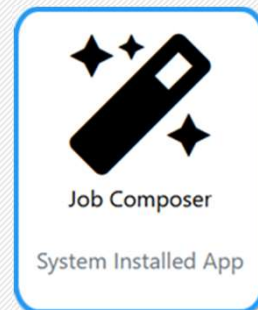
- View
- Edit
- Upload
- Download files



Starting a Job

OnDemand allows users to:

- Create
- Edit
- Submit
- Monitor jobs



CSKK's Open OnDemand / Job Composer Jobs Templates Help

Jobs

+ New Job

Edit Files Job Options Open Terminal

Show 25 entries Search:

Created	Name	ID	Cluster	Status
June 11, 2023 12:05pm	(default) Simple Sequential Job		PBS	Not Submitted

Showing 1 to 1 of 1 entries Previous 1 Next

Job Details

Job Name:
(default) Simple Sequential Job


Submit to:
PBS

Account:
Not specified

Script location:
/nfs/home/gutmann/ondemand/data/sys/myjobs/projects/c

Script name:
main_job.sh

Folder Contents:
main_job.sh



Cluster	Status
PBS	Not Submitted
Previous 1 Next	

Starting a Job

OnDemand allows users to:

- Create
- Edit
- Submit
- Monitor jobs

The screenshot displays the CSK's Open OnDemand Job Composer interface. At the top, a green notification bar states "Job was successfully submitted." Below this, the "Jobs" section shows a table with one job entry. A red arrow points from the "Running" status of this job in the table to a detailed view of the job on the right.

Jobs Table:

Created	Name	ID	Cluster	Status
June 11, 2023 12:05pm	(default) Simple Sequential Job	94.sakura-server	PBS	Running

Showing 1 to 1 of 1 entries

Job Details:

94.sakura-server
Job Name:
(default) Simple Sequential Job

Submit to:
PBS

Account:
Not specified

Script location:
/nfs/home/gutmann/ondemand/data/sys/myjobs/projects/c

Script name:
main_job.sh

Folder Contents:

Completed Job

OnDemand allows users to:

- Create
- Edit
- Submit
- Monitor jobs

The screenshot displays the CSKK's Open OnDemand Job Composer interface. At the top, a green notification bar states "Job was successfully submitted." Below this, the "Jobs" section features a table with columns: Created, Name, ID, Cluster, and Status. A single job is listed: "94.sakura-server" with ID "94.sakura-server", Cluster "PBS", and Status "Completed". A red arrow points from this job entry to a detailed view on the right. The detailed view shows the job name "94.sakura-server", a "(default) Simple Sequential Job", and fields for "Submit to:" (PBS), "Account:" (Not specified), "Script location:" (a file path), "Script name:" (main_job.sh), and "Folder Contents:".

CSKK's Open OnDemand / Job Composer Jobs Templates Help

Job was successfully submitted.

Jobs

+ New Job

Edit Files Job Options Open Terminal

Show 25 entries Search:

Created	Name	ID	Cluster	Status
June 11, 2023 12:05pm	(default) Simple Sequential Job	94.sakura-server	PBS	Completed

Showing 1 to 1 of 1 entries Previous 1 Next

Job Details

94.sakura-server

Job Name:

(default) Simple Sequential Job

Submit to:

PBS

Account:

Not specified

Script location:

/nfs/home/gutmann/ondemand/data/sys/myjobs/projects/

Script name:

main_job.sh

Folder Contents:

Job Results

OnDemand allows users to:

- Create
- Edit
- Submit
- Monitor jobs

The screenshot displays the CSKK's Open OnDemand Job Composer interface. At the top, a green notification bar states "Job was successfully submitted." Below this, the "Submit Script" section shows the script content for "main_job.sh":

```
#!/bin/bash
# JOB HEADERS HERE

echo "Hello World"
```

At the bottom of the "Submit Script" section, there are three buttons: "Open Editor", "Open Terminal", and "Open Dir". The "Open Dir" button is highlighted with a red rectangle. A blue arrow points from the "Open Dir" button to a smaller inset window on the right. This inset window shows the "Job Details" for job ID "94.sakura-server", which is in a "Completed" state. The "Job Details" section includes fields for "Job Name", "Submit to", "Account", "Script location", "Script name", and "Folder Contents". The "Folder Contents" section lists "STDIN.op4" and "main_job.sh". At the bottom of the inset window, there is a "Submit Script" section with the same script content as the main window, and buttons for "Open Editor", "Open Terminal", and "Open Dir".

Previewing the Output

- Results can be previewed in the browser
- GUI makes it easy if there are many outputs in one or more directories

このOpen OnDemandは開計算科学のポータルページです。

Open in Terminal Refresh New File New Directory Upload Download Copy/Move Delete

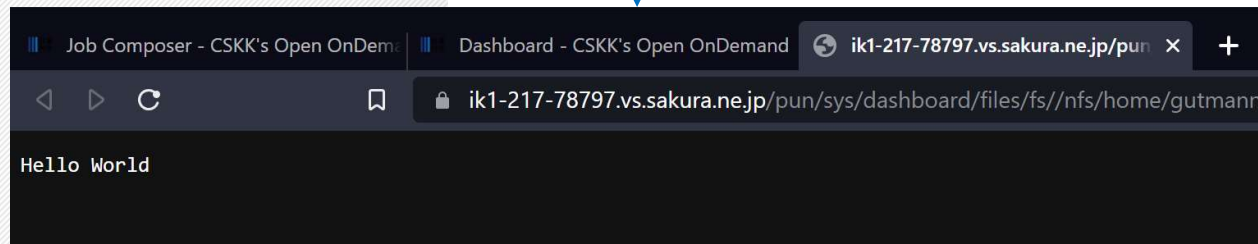
Home Directory

↑ / nfs / home / gutmann / ondemand / data / sys / myjobs / projects / default / 1 / Change directory Copy path

☐ Show Owner/Mode ☐ Show Dotfiles Filter: Showing 2 rows - 0 rows selected

Type	Name	Size	Modified at
<input type="checkbox"/>	main_job.sh	51 Bytes	6/11/2023 12:05:30 PM
<input type="checkbox"/>	STDIN.o94	12 Bytes	6/15/2023 9:30:25 AM

OnDemand version: latest



Jupyter Notebooks

Jupyter is one of the main tools for prototyping AI and other work



CSKK's Open OnDemand Apps Files Jobs Clusters Interactive Apps My Interactive Sessions ヘルプ Logged in as gutmann ログアウト

Home / My Interactive Sessions / Jupyter Notebook

Interactive Apps

- Desktops
- My Cluster Desktop(VNC 接続)
- GUIs
- COMSOL Multiphysics
- Servers
- Jupyter Notebook**

Jupyter Notebook

This app will launch a Jupyter Notebook server on one or more nodes.

Mode

Modules

Account

実行時間

☒ 1 ☐ 2

Queue

Number of hours

Number of nodes

☐ I would like to receive an email when the session starts

Launch

* The Jupyter Notebook session data for this session can be accessed under the data root directory.

powered by **OPEN OnDemand**

OnDemand version: latest

Jupyter Notebooks: Launching

You can specify:

- Mode
- Modules
- Account
- Time
- Queue name
- Node count
- Email alerts



CSKK's Open OnDemand Apps Files Jobs Clusters Interactive Apps My Interactive Sessions ヘルプ Logged in as gutmann ログアウト

Home / My Interactive Sessions / Jupyter Notebook

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Jupyter Notebook

This app will launch a Jupyter Notebook server on one or more nodes.

Mode

Modules

Account

実行時間
☒ 1 ☐ 2

Queue

Number of hours

Number of nodes

☐ I would like to receive an email when the session starts

* The Jupyter Notebook session data for this session can be accessed under the data root directory.

powered by **OPEN OnDemand**

OnDemand version: latest

Jupyter Notebooks: Launching

You can specify:

- Mode
- **Modules**
- Account
- Time
- Queue name
- Node count
- Email alerts

The screenshot shows the 'Jupyter Notebook' launch page in the CSKK's Open OnDemand portal. The page has a purple header with navigation links: Home, My Interactive Sessions, Jupyter Notebook, Apps, Files, Jobs, Clusters, Interactive Apps, and My Interactive Sessions. The user is logged in as 'gutmann' and can log out. The left sidebar shows a list of interactive apps: Desktops, My Cluster Desktop(VNC 接続), GUIs, COMSOL Multiphysics, and Servers. The main content area is titled 'Jupyter Notebook' and includes a description: 'This app will launch a Jupyter Notebook server on one or more nodes.' Below this are input fields for 'Mode', 'Modules' (containing 'pandas, numpy, matplotlib, scipy, mpmath, sklearn'), and 'Account' (containing 'gutmann'). There is also a '実行時間' (Execution Time) field with a value of '1'. At the bottom, there is a checkbox for 'I would like to receive an email when the session starts' and a 'Launch' button. A footer note states: '* The Jupyter Notebook session data for this session can be accessed under the data root directory.' The page is powered by 'OPEN OnDemand' and the version is 'latest'.

CSKK's Open OnDemand Apps Files Jobs Clusters Interactive Apps My Interactive Sessions ヘルプ Logged in as gutmann ログアウト

Home / My Interactive Sessions / Jupyter Notebook

Interactive Apps

- Desktops
- My Cluster Desktop(VNC 接続)
- GUIs
- COMSOL Multiphysics
- Servers
- Jupyter Notebook**

Jupyter Notebook

This app will launch a Jupyter Notebook server on one or more nodes.

Mode

Modules

pandas, numpy, matplotlib, scipy, mpmath, sklearn

Account

gutmann

実行時間

1

Modules

pandas, numpy, matplotlib, scipy, mpmath, sklearn

☐ I would like to receive an email when the session starts

Launch

* The Jupyter Notebook session data for this session can be accessed under the data root directory.

powered by OPEN OnDemand

OnDemand version: latest

Interactive Session List

Can view:

- Active notebooks
- Past notebooks

Can access the:

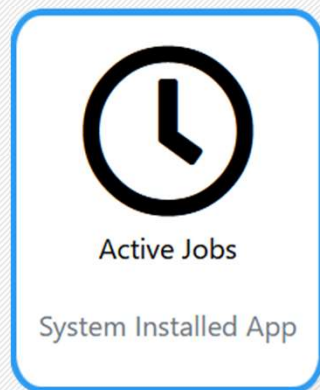
- Notebook itself
- Notebook's host terminal
- Session

The screenshot displays the CSKK's Open OnDemand web interface. The top navigation bar includes links for Apps, Files, Jobs, Clusters, Interactive Apps, and My Interactive Sessions, along with a help icon and user information (Logged in as gutmann). A yellow banner at the top states: "このOpen OnDemandは情報科学のポータルページです。". A green notification bar indicates "Session was successfully created." Below this, the breadcrumb "Home / My Interactive Sessions" is shown. On the left, a sidebar titled "Interactive Apps" lists Desktops, My Cluster Desktop(VNC 接続), GUIs, COMSOL Multiphysics, Servers, and Jupyter Notebook. The main content area shows a list of interactive sessions. The first session, "Jupyter Notebook (98.sakura-server)", is in a "Running" state with 1 node and 1 core. It shows the host as "sakura-client2", created at "2023-06-15 06:00:30 UTC", with 1 minute remaining. The session ID is "a0a6fd0e-2f3c-4f5a-a5ec-03eebe187501". A "Connect to Jupyter" button is available. The second session, "Jupyter Notebook (97.sakura-server)", is in a "Completed" state, created at "2023-06-15 05:52:39 UTC", with session ID "9b8a382f-76d3-49d1-bf0f-18c4bf51f39a". A "Delete" button is present. A note at the bottom states: "For debugging purposes, this card will be retained for 6 more days".

Active Job Monitoring

Can view all jobs running

- Interactive jobs
- Batch jobs



CSKK's Open OnDemand Apps Files Jobs Clusters Interactive Apps

このOpen OnDemandは(株)計算科学のポータルページです。

Your Jobs All Clusters

Active Jobs

Show 50 entries Filter:

ID	Name	User	Account	Time Used	Queue	Status	Cluster	Actions
> 98.sakura-server	Jupyter.ood	gutmann	gutmann	00:00:26	workq	Running	PBS	

Showing 1 to 1 of 1 entries

Previous 1 Next

powered by OPEN OnDemand

OnDemand version: latest

Active Job Monitoring

Can view all jobs running

- Interactive jobs
- Batch jobs


CSKK's Open OnDemand Apps Files Jobs Clusters Interactive Apps

このOpen OnDemandは(仮)計算科学のポータルページです。

Your Jobs All Clusters

Active Jobs

Show 50 entries Filter:

ID	Name	User	Account	Time Used	Queue	Status	Cluster	Actions	
>	98.sakura-server	Jupyter.ood	gutmann	gutmann	00:00:26	workq	Running	PBS	

powered by OPEN OnDemand

OnDemand version: latest

Virtual Desktop

Can use applications that only have a GUI interface
That do not have Open OnDemand support yet



CSKK's Open OnDemand Apps Files Jobs Clusters Interactive Apps My Interactive Sessions ヘルプ Logged in as ログアウト

このOpen OnDemandは数値計算科学のポータルページです。

Home / My Interactive Sessions / My Cluster Desktop(VNC 接続)

Interactive Apps

- Desktops
- My Cluster Desktop(VNC 接続)**
- GUIs
- COMSOL Multiphysics
- Servers
- Jupyter Notebook

My Cluster Desktop(VNC 接続)

日本語のテストです。ここはCSKKのOpenOnDemandのテストページです。

Account

gutmann

Number of hours

1

Number of nodes

1

Queue

workq

☐ I would like to receive an email when the session starts

Launch

* The My Cluster Desktop(VNC 接続) session data for this session will be stored under the data root directory.

powered by OPEN OnDemand

OnDemand version: latest

TurboVNC viewer window showing a desktop environment with icons for Trash, Home, and File System. The desktop background is blue. The window title bar shows "TurboVNC viewer" and "Applications". The system tray at the bottom shows the date and time: "Wed 14 Jun, 14:25".