計算科学
Computational Science Inc.

Open On Demand

About Me: Greg Gutmann

Past

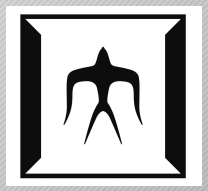
- NASA Goddard Space Flight Center (2013-2015)
- Tokyo Institute of Technology: PhD (2016)
- Tokyo Institute of Technology: Assistant Professor (2017-2022)

Present

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

Focus

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



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

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https://www.linkedin.com/in/greg-gutmann-b0639255

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

https://www.awesim.org/products

- TotalSim US one of the largest OSC OnDemand users
  - Focused on CFD simulation

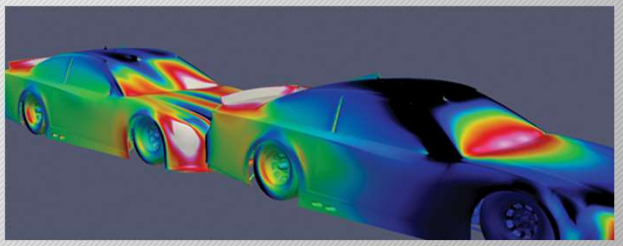
https://totalsim.us/

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*

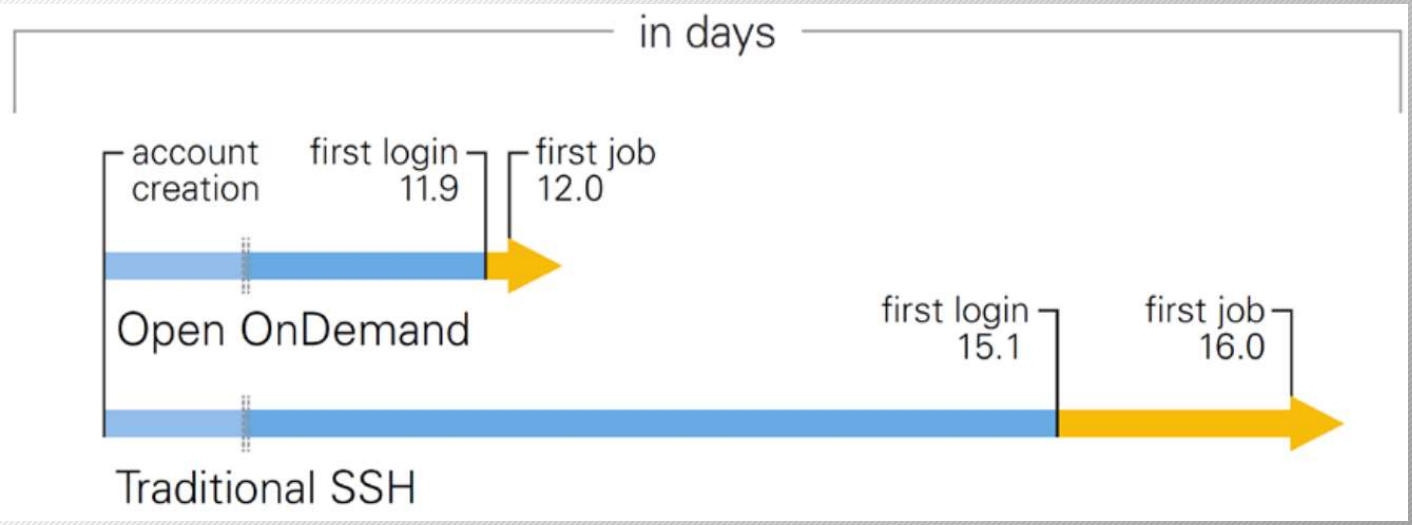
https://www.hpcwire.com/2020/12/21/ondemand-portal-accelerates-hpc-work-for-academic-and-industrial-users/
https://www.osc.edu/research/research-reports/2020/fluid_dynamics

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*

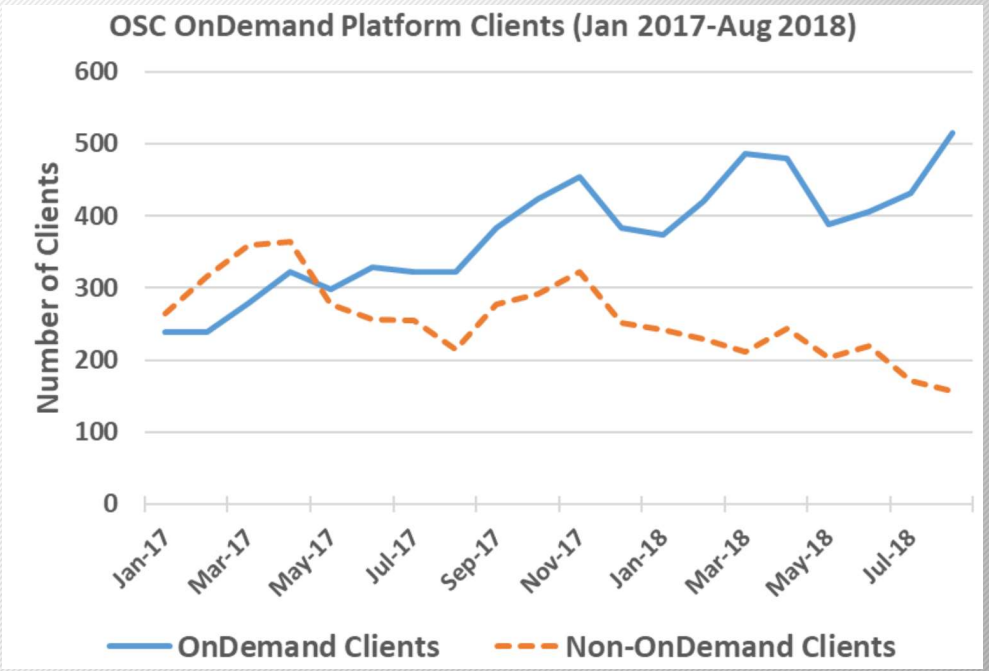
* https://www.nitrd.gov/nitrdgroups/images/c/cb/MAGIC-2019-06-Alan-Chalker.pdf

OnDemand User Study
from The Ohio Supercomputer Center

- OSC saw a steady migration from:

Non-OnDemand clients

OnDemand clients



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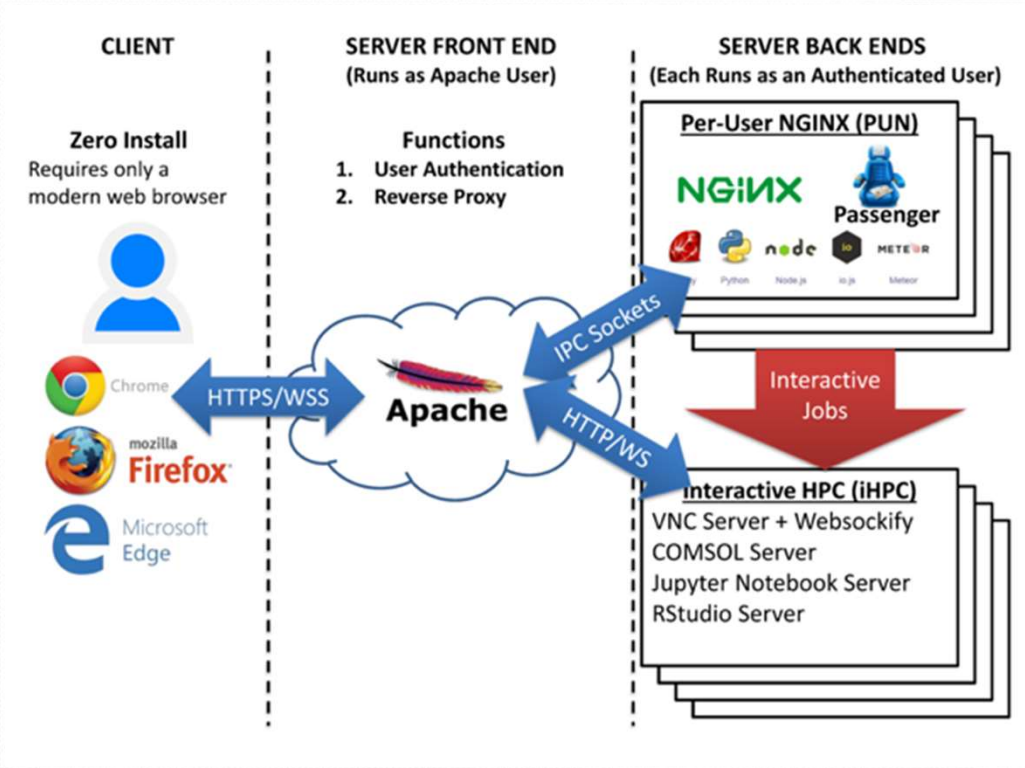
Architecture & Security

Architecture Overview

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

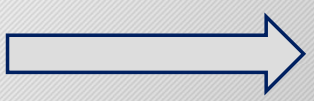


https://osc.github.io/ood-documentation/latest/architecture.html

Security measures

- HTTPS / SSL ---- *Encrypted connections*
- Firewall --------- *Network traffic control*
- LDAP ------------ *Secure resource access*
- Reverse Proxy -- *Eliminates direct communication to server*

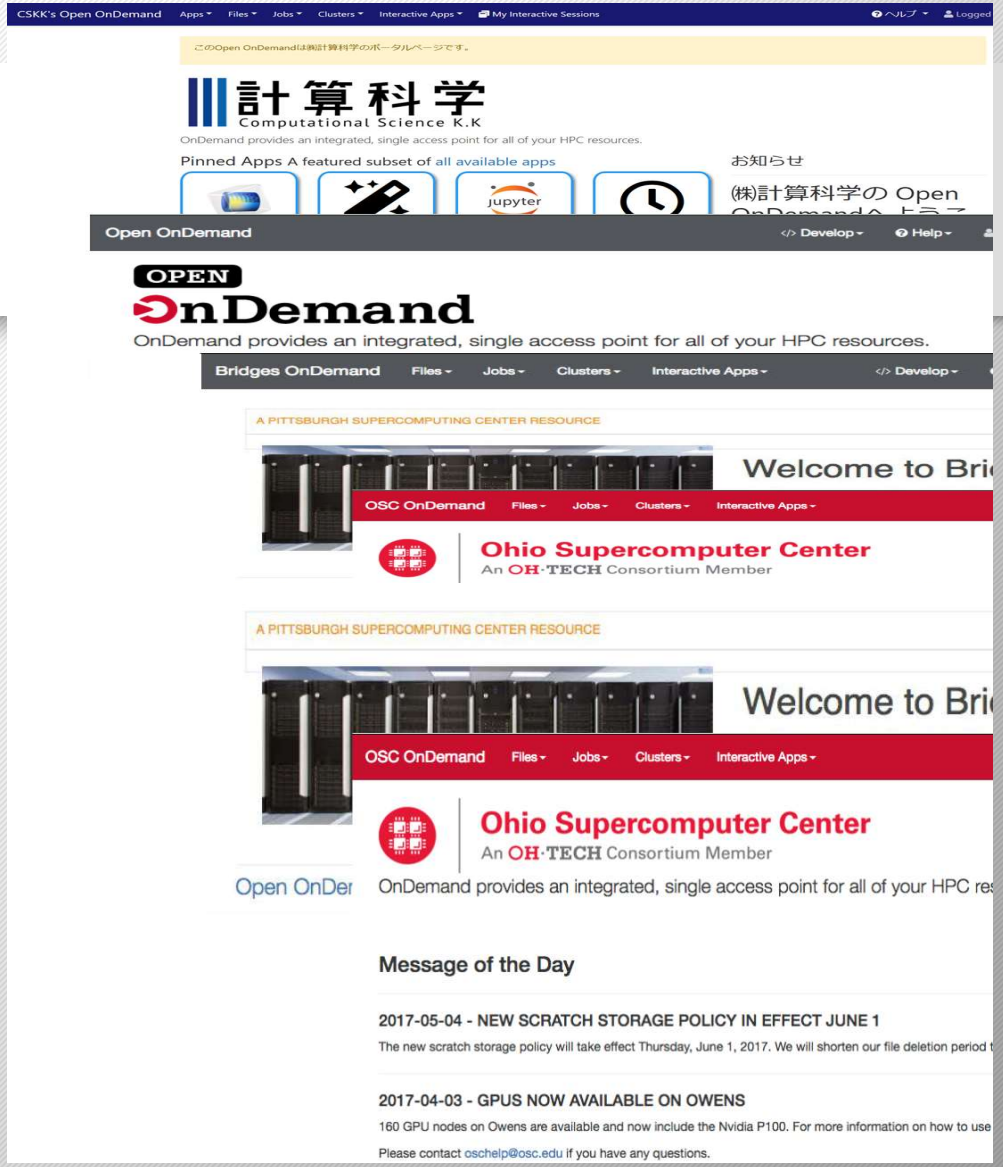
- Login authentication with OpenID
  - Third-party identity provider (IDP) service
  - Eliminating the need for webmasters to provide their own ad hoc login systems



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

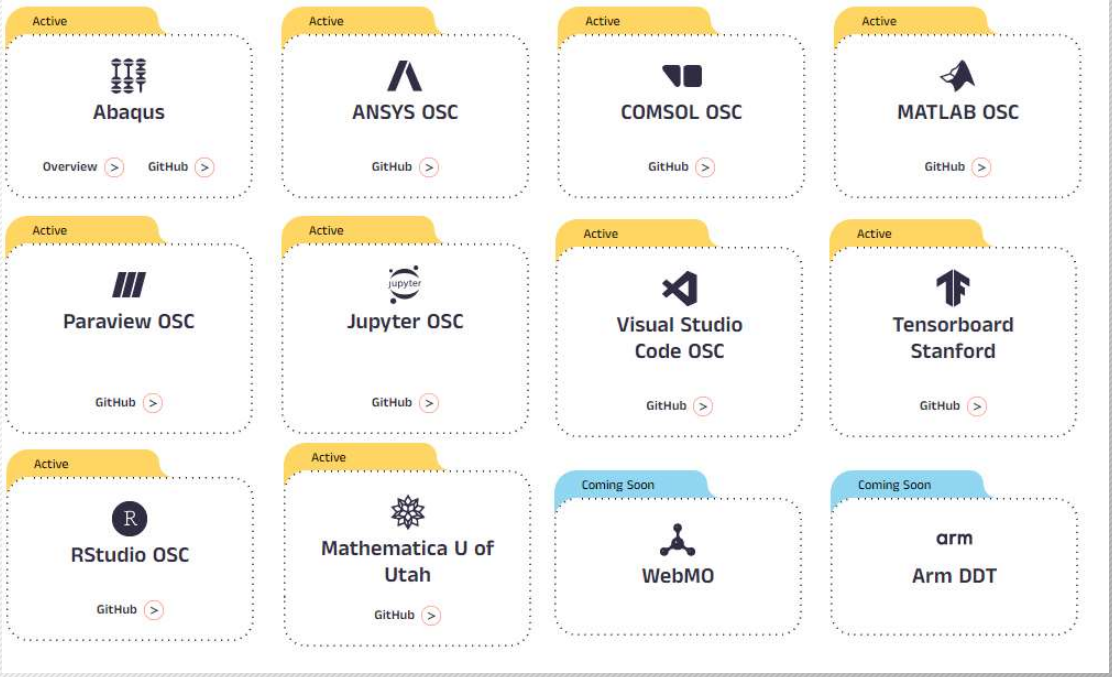
- PBS Pro
- SLURM
- Grid Engine
- Torque
- LSF

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

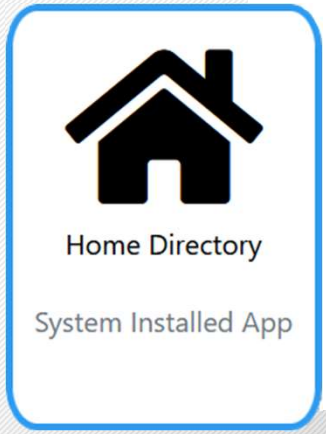
Live Demonstration

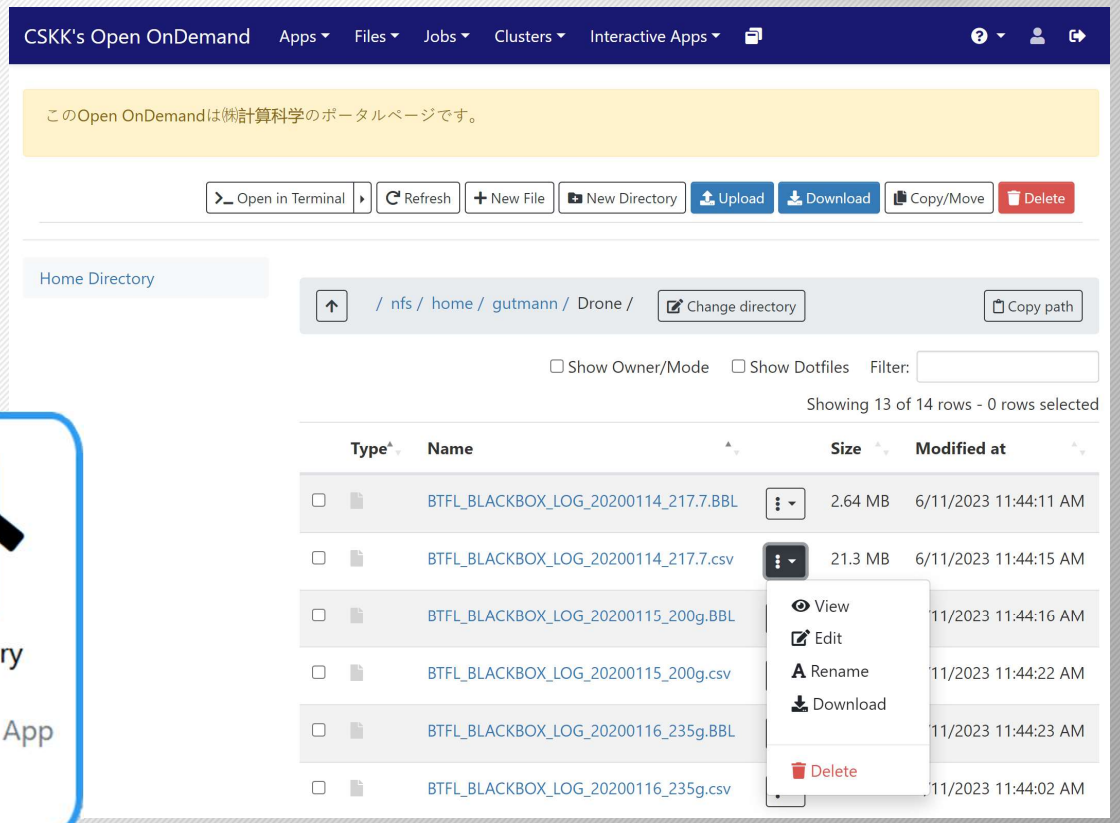
Offline Demonstration

Home Directory

OnDemand allows users to:

- View
- Edit
- Upload
- Download files





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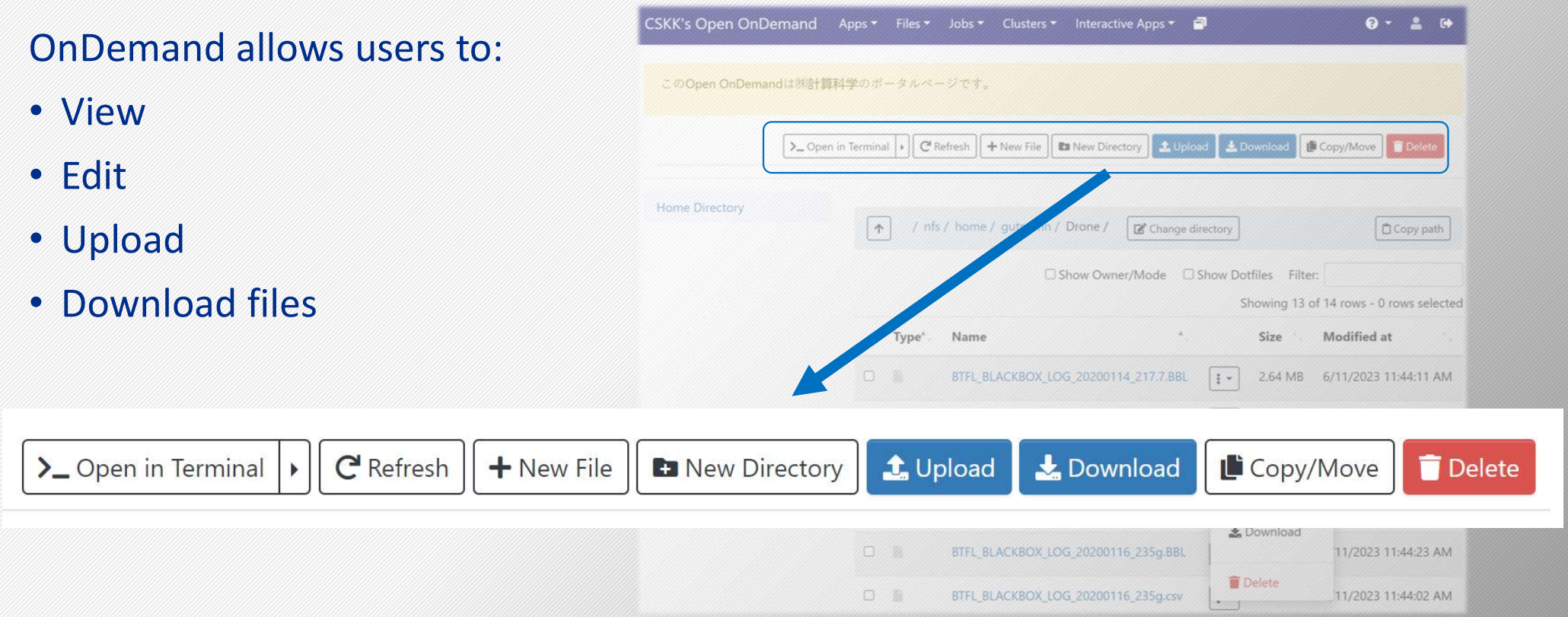

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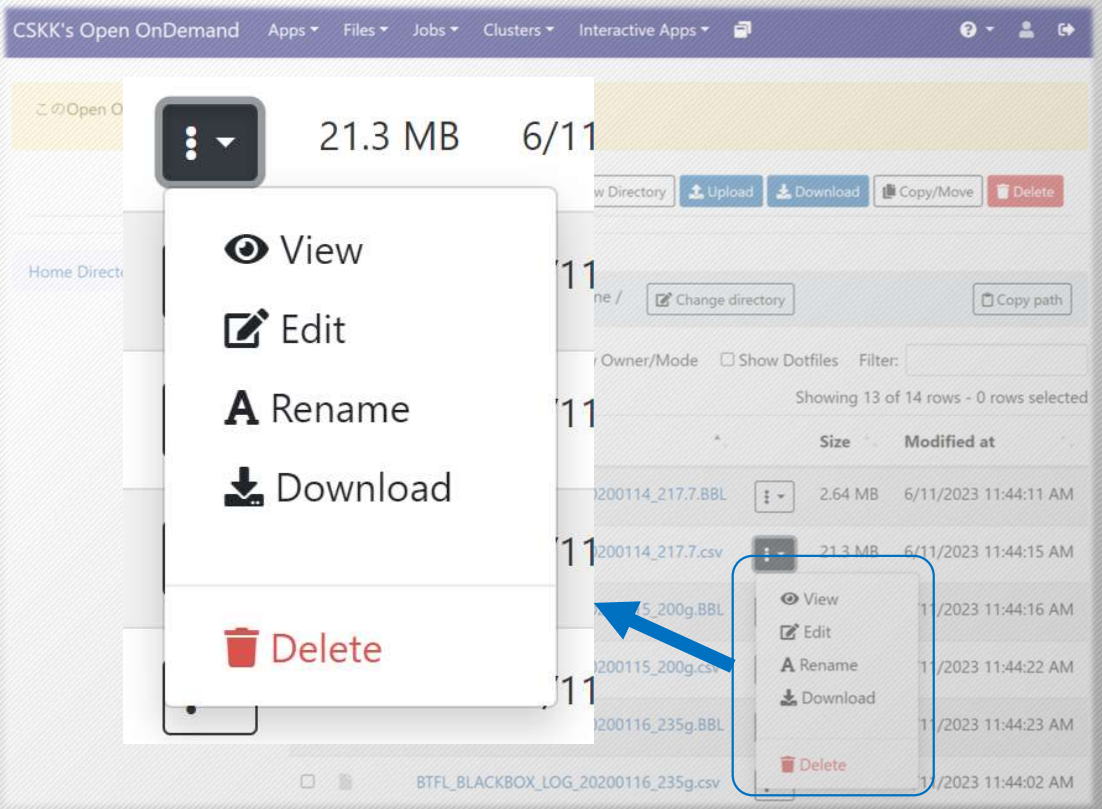
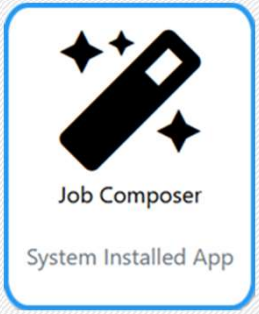
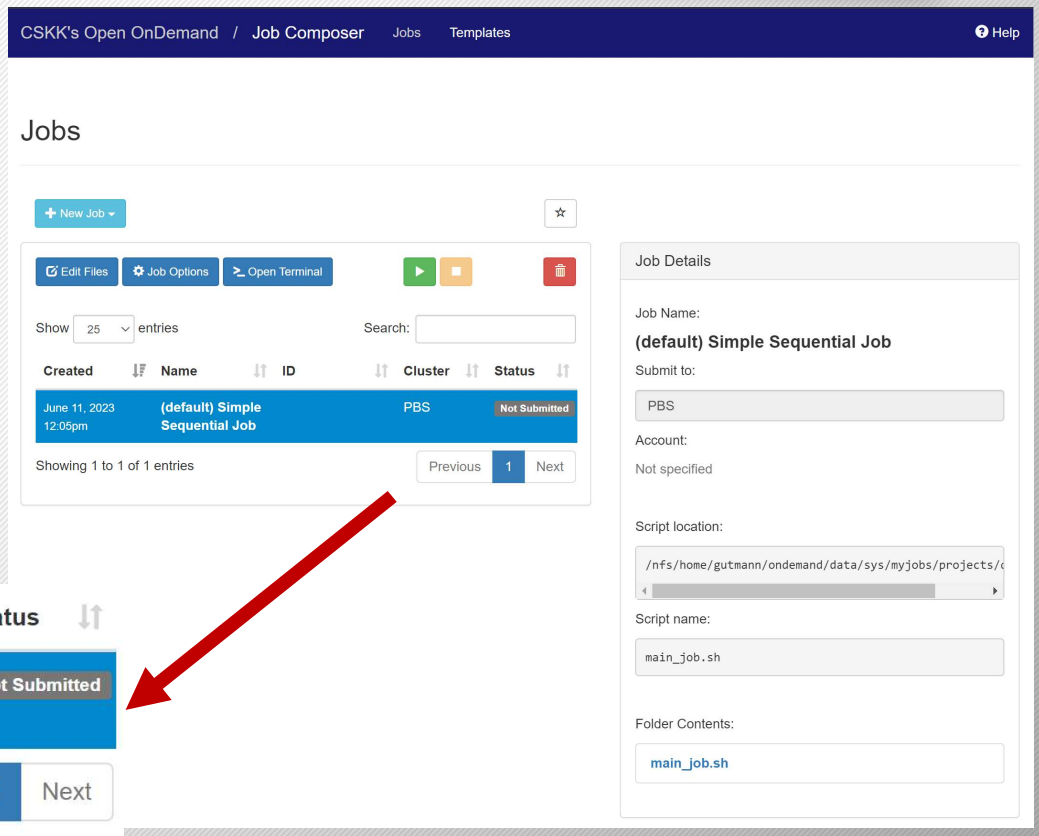


Starting a Job

OnDemand allows users to:

- Create
- Edit
- Submit
- Monitor jobs





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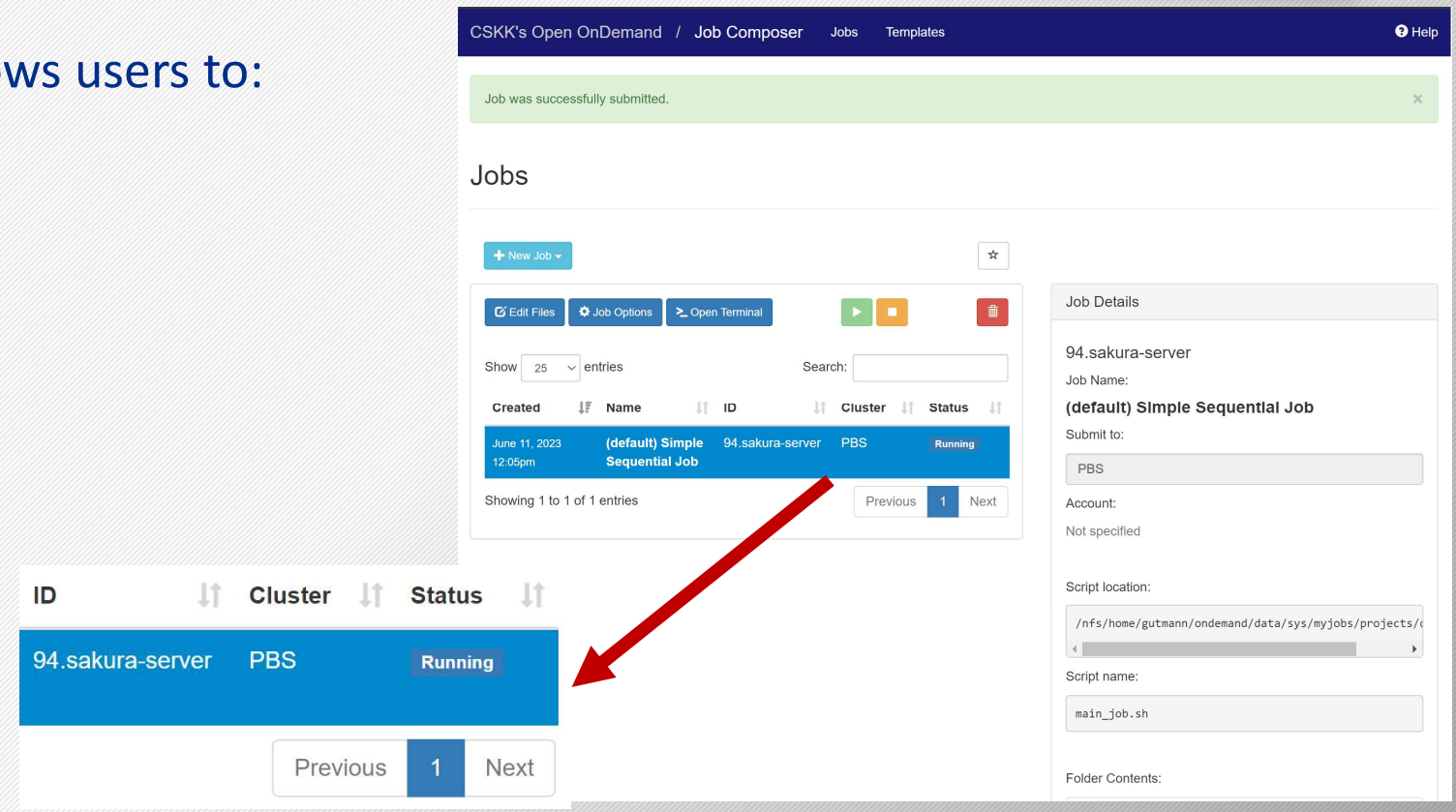
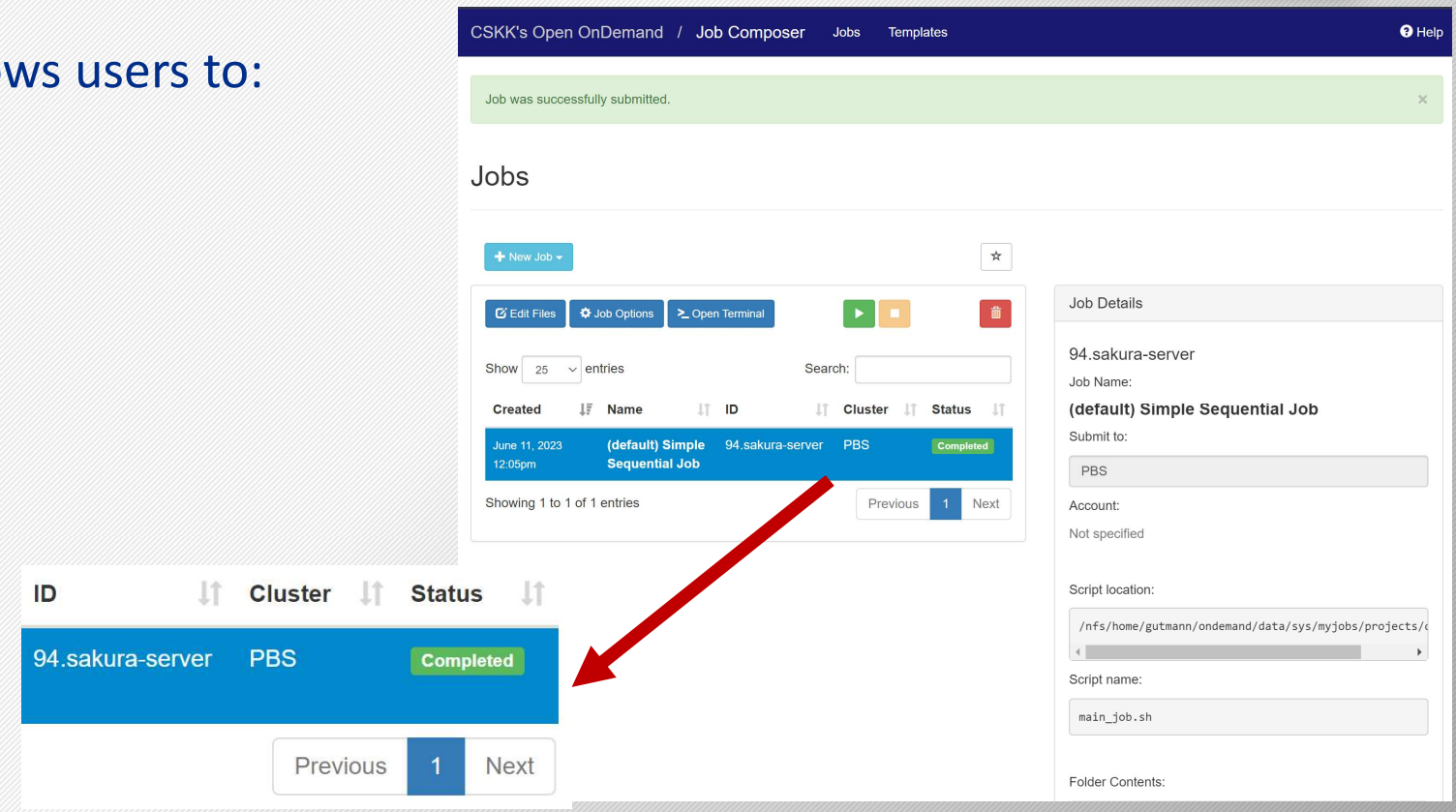


Completed Job

OnDemand allows users to:

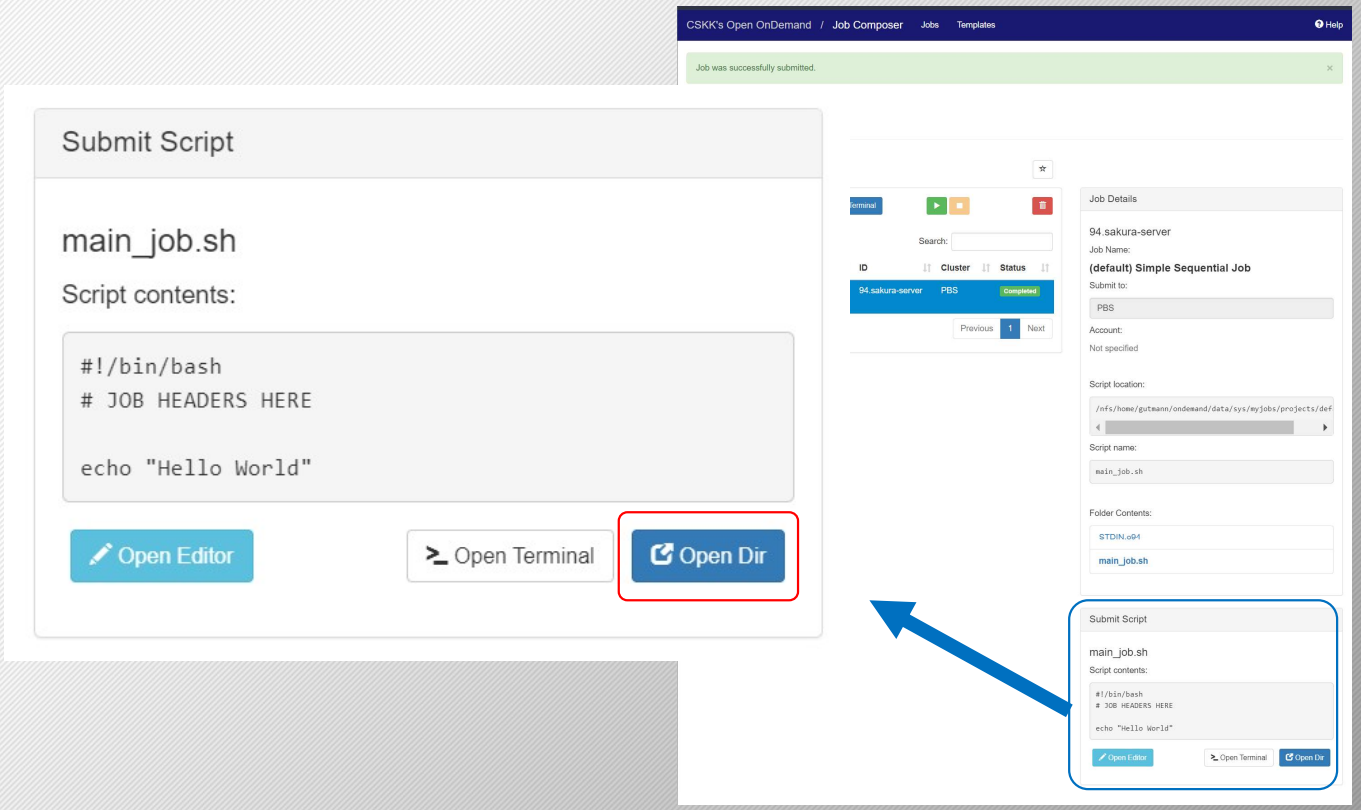
- Create
- Edit
- Submit
- Monitor jobs



Job Results

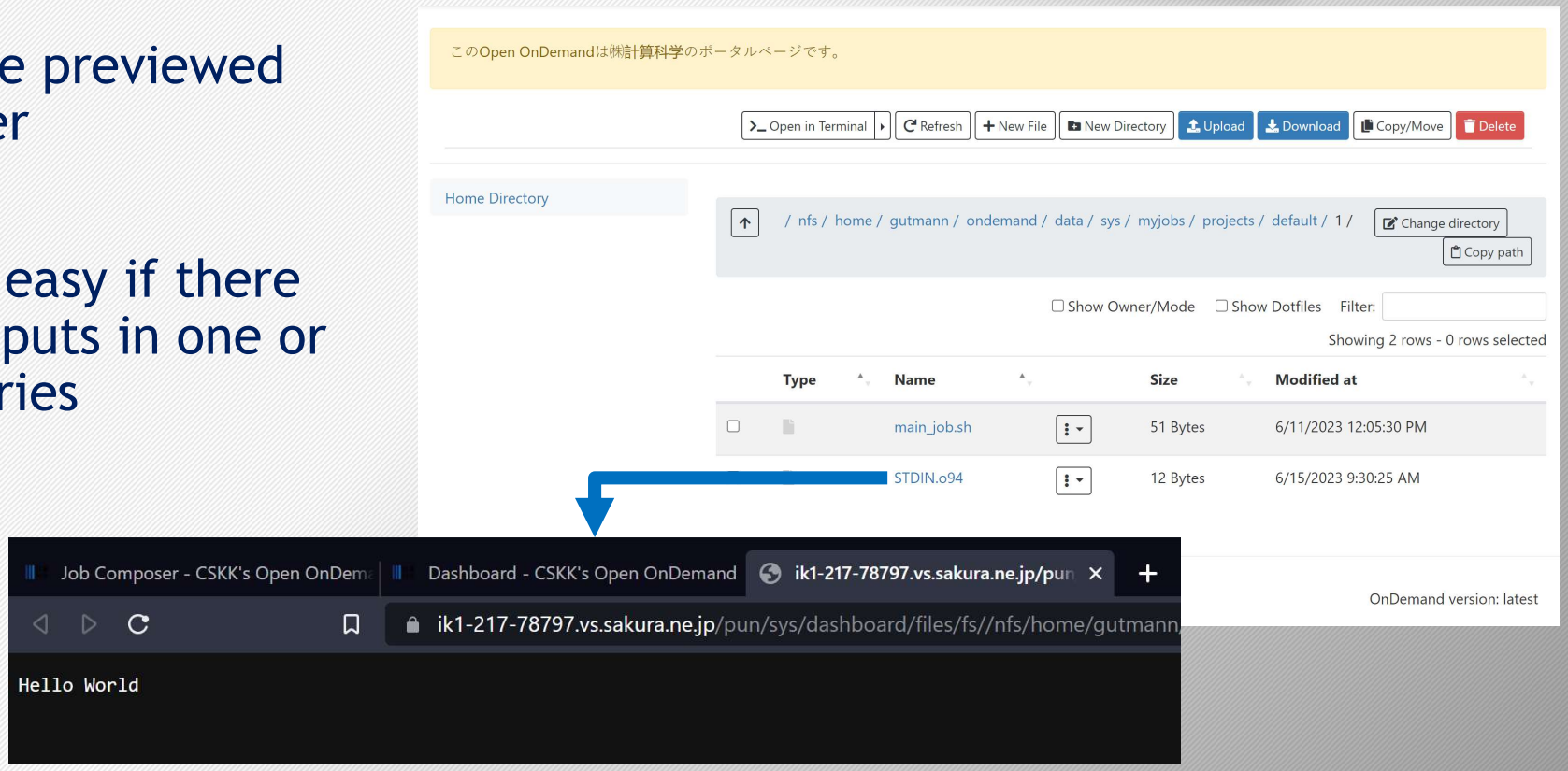
OnDemand allows users to:

- Create
- Edit
- Submit
- Monitor jobs



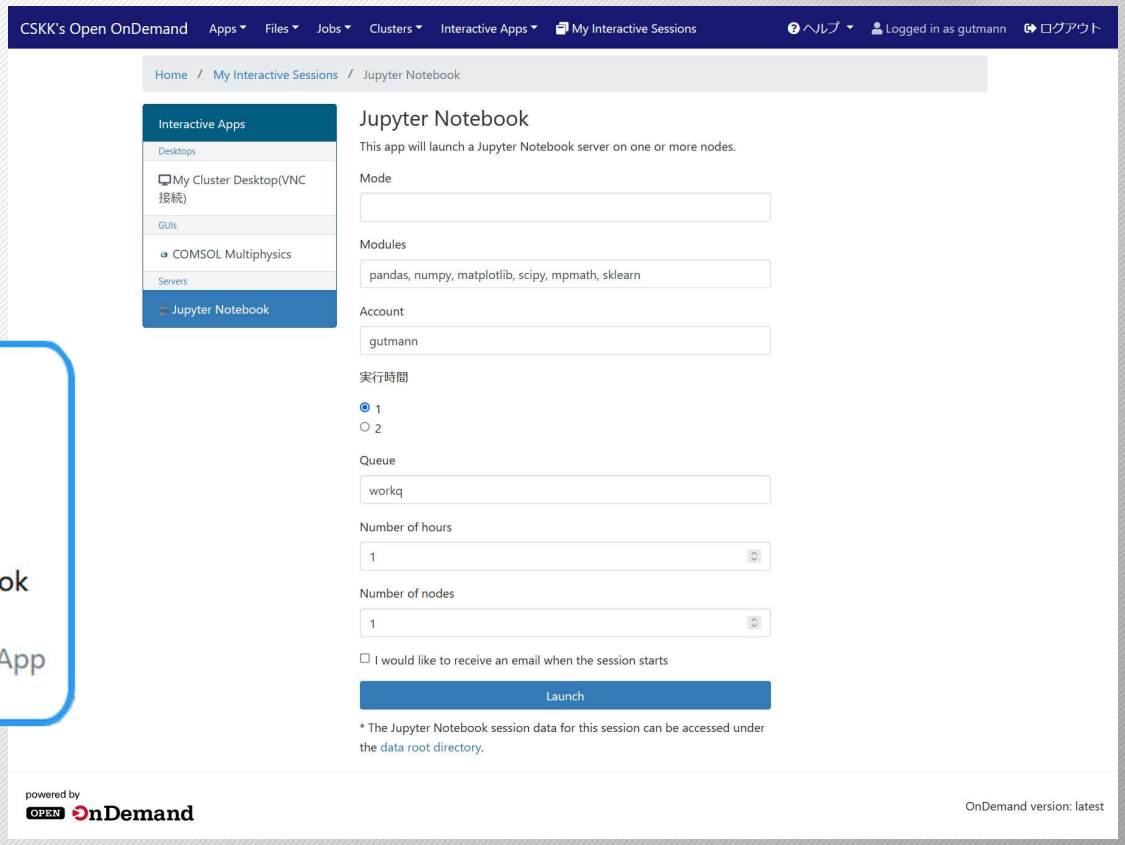
Previewing the Output

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



Jupyter Notebooks

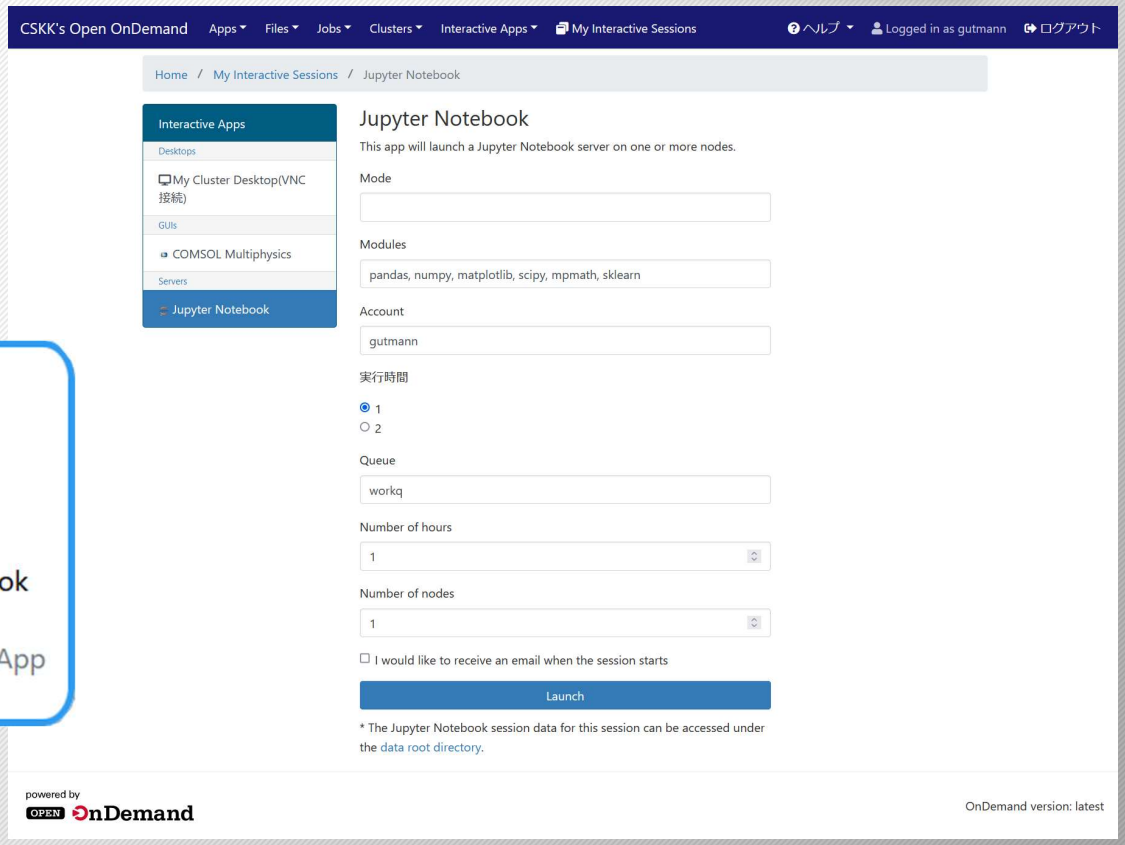
Jupyter is one of the main tools for prototyping AI and other work



Jupyter Notebooks: Launching

You can specify:

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



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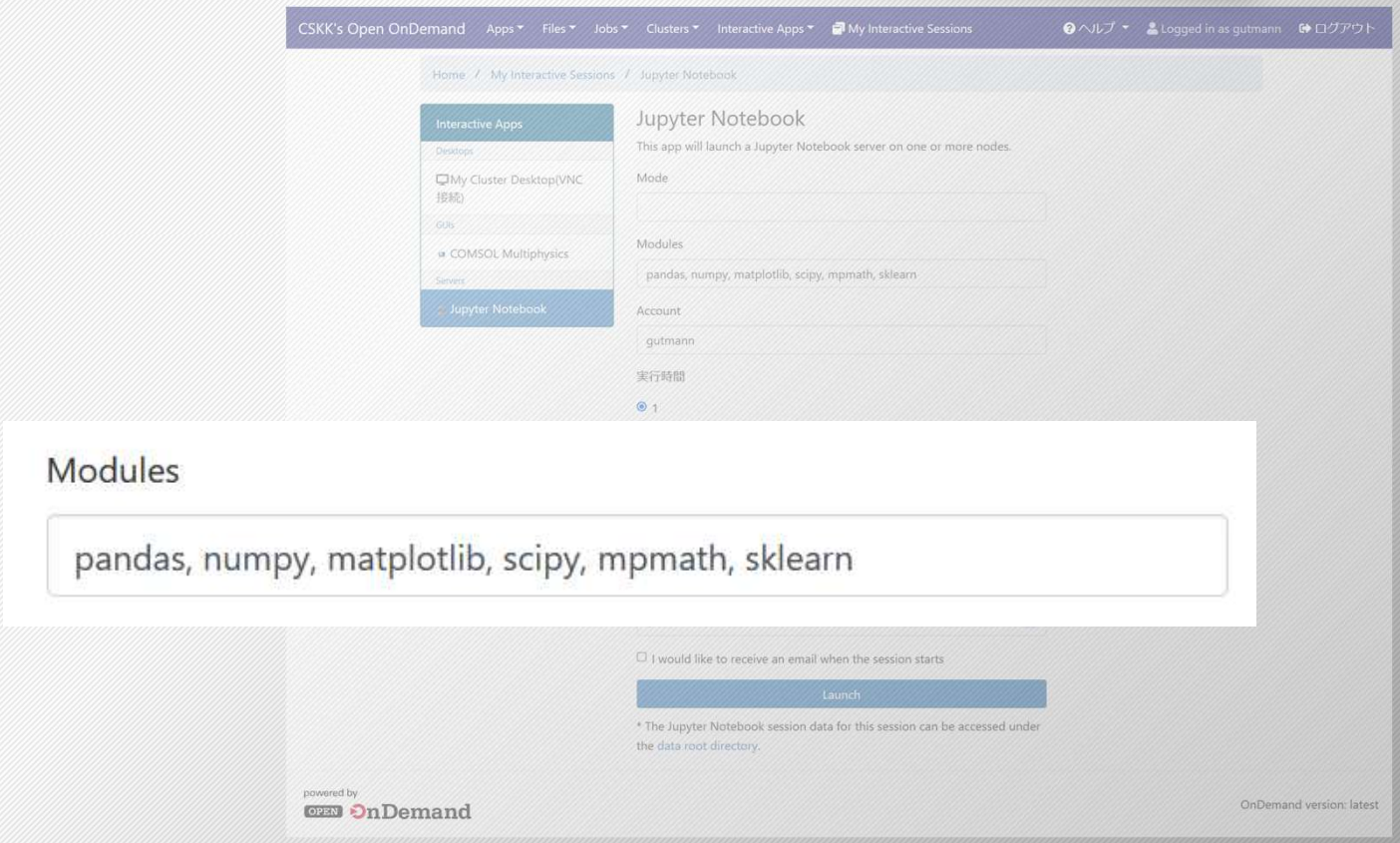


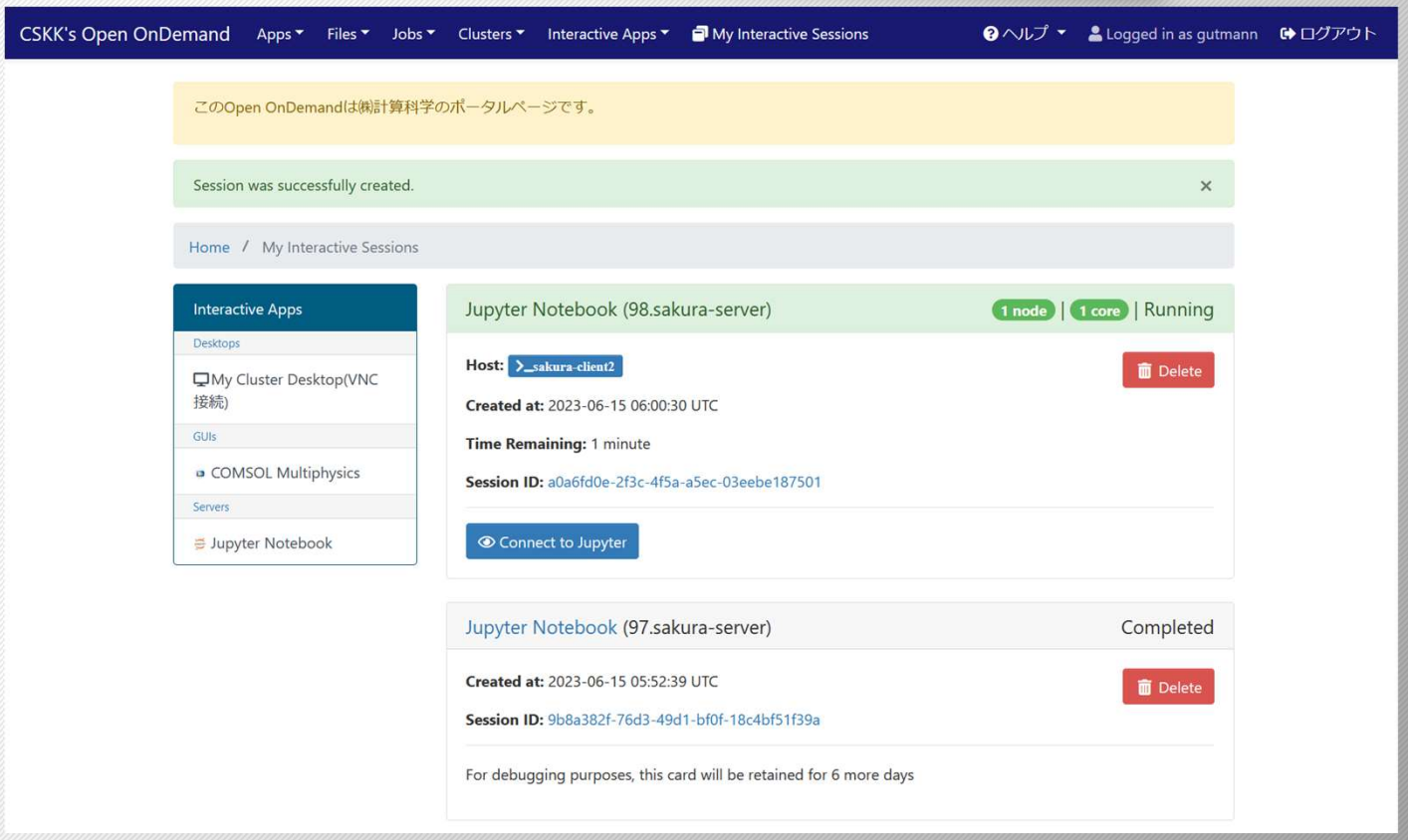
Interactive Session List

Can view:

- Active notebooks
- Past notebooks

Can access the:

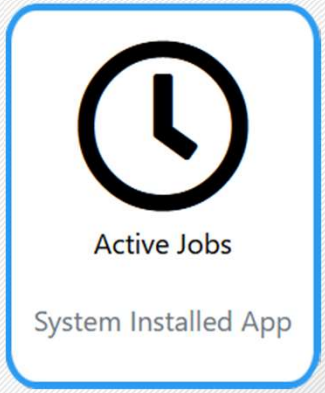
- Notebook itself
- Notebook’s host terminal
- Session

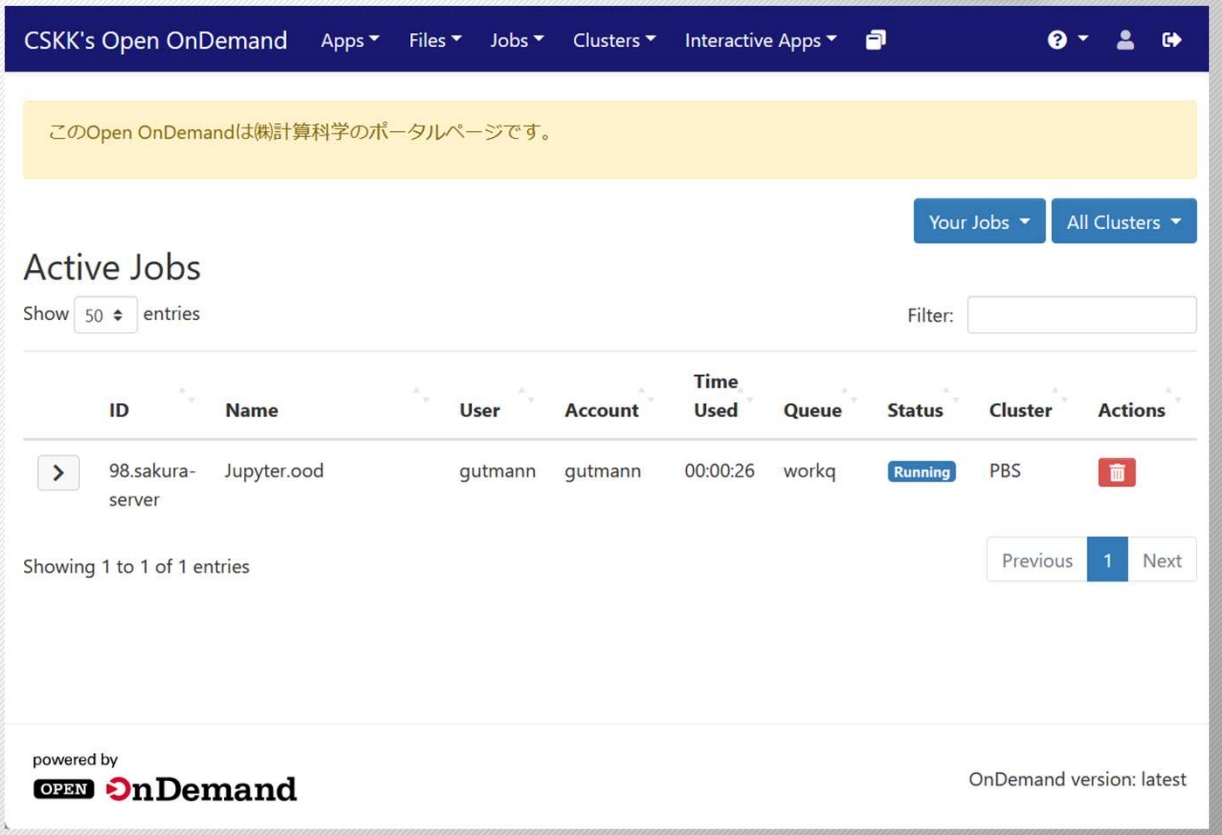


Active Job Monitoring

Can view all jobs running

- Interactive jobs
- Batch jobs





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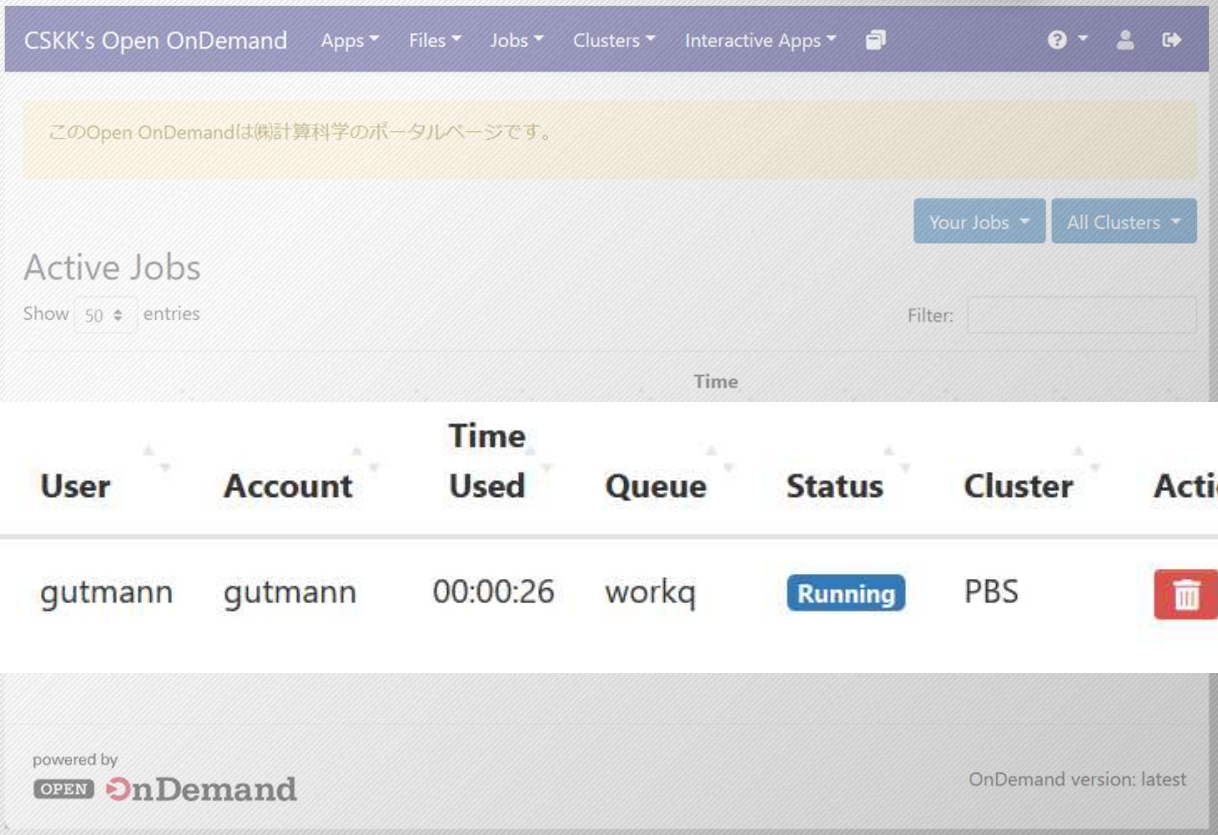

Virtual Desktop

Can use applications that only have a GUI interface

That do not have Open OnDemand support yet