Introduction to Interactive HPC

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What is Interactive Computing?

Interactive Computing is about immediacy. When the human requests an action, the computer immediately responds. When the computer finishes a task, the human immediately perceives the result.

- Software GUIs
- Prototyping workflows
  - Design your workflow for a single node (multi-core) or small set of nodes
  - Discover and test new tools/concepts
  - Profile, optimize and debug
- Data Visualization

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Why Interactive HPC?

HPC is part of a larger research workflow

Dr. so-and-so needs to explore a huge dataset

Needs: interactivity, analytics tools, large memory/storage

Dr. such-and-such is preparing to create a cutting-edge simulation visualization

Needs: interactivity, remote visualization, compute, bandwidth

A grad student is prototyping a new algorithm

Needs: interactivity, dev and debug tools, time to iterate

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Tutorial Outline

- Batch vs. Interactive Computing @ MSI
- Getting Started with Interactive Resources
  - Connecting to MSI
  - Conscientious Computing
  - Prototyping Workflows
- Hands-on
  - Remote desktops
  - Jupyter Notebooks

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MSI Access Overview

Researcher

Needs compute resources

Secure Network

On-campus eduroam or ethernet
Off-campus via UMN VPN

MSI Access Gateway

OnDemand Portal
SSH Command Line
Other Web Portals

HPC Compute

Computation on MSI clusters
Agate, Mangi, Mesabi

Data Storage

Primary - Home+Project Dirs
2nd Tier - object storage
Scratch storage areas

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Resource Allocations

ALL groups will have access to these basic resources:

- High Performance Computing cluster access
- High Performance Storage
  - 150 GB home directory quota or more if requested
  - Home and project storage accessible from most MSI systems
- Access to interactive gateways
- Access to MSI labs
  - contact us to activate your Ucard for physical access

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Survey of Options

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Batch Jobs

- When should you use Batch Jobs?
  - *Whenever possible!* This is the traditional way to work in HPC
  - Share resources and be considerate of other researchers
- What are the benefits of Batch Jobs?
  - Headless execution of automated processes
  - Long runtimes
  - Large core counts
  - A scheduler packs jobs in hardware to maximize utilization, reduce latency, etc.

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Interactive Options

- **OnDemand Portal**
- **Interactive batch** (srun via the command line)
- **Jupyter portal** (sharable reproducible computing)
- **Galaxy portal** (graphically compose workflows)
- Specialized solutions
  - CITRIX for Windows apps
  - Stratus “private cloud” instances

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OnDemand Portal

https://ondemand.msi.umn.edu

- **OnDemand Web Portal is a new offering in 2022**
- One-stop access portal for interactive HPC services
  - Remote desktop access
  - Command line terminal
  - File browser
  - Launchers for common GUI scientific applications
  - JupyterLab server access
  - RStudio server access

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Interactive Command Line

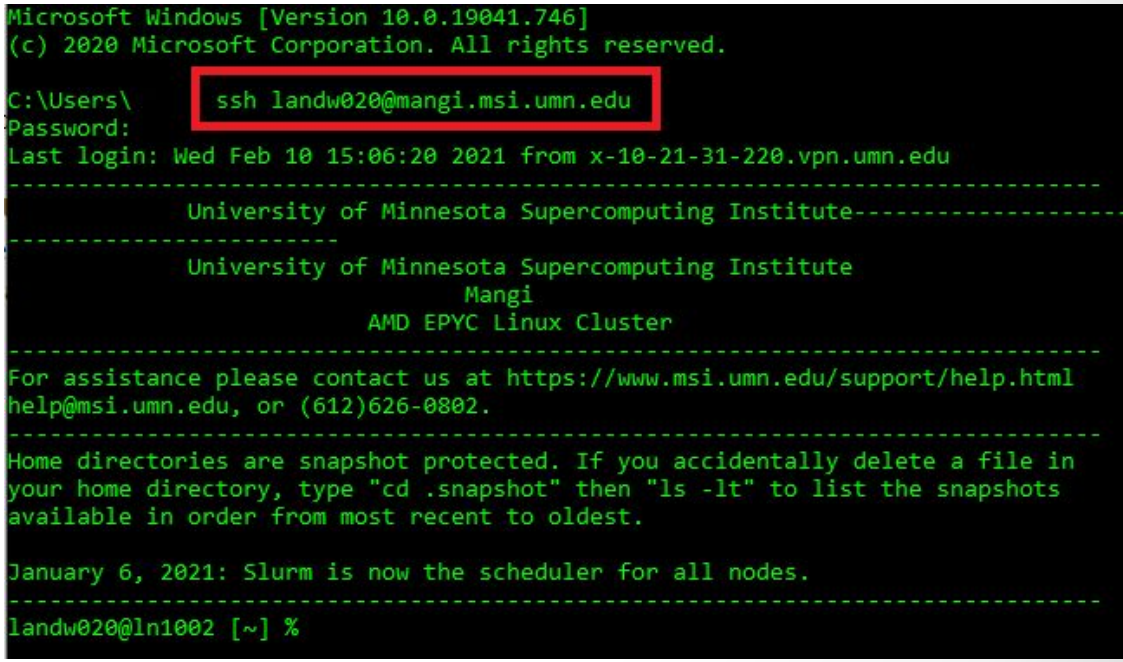
ssh <username>@<resource>.msi.umn.edu

See: https://www.msi.umn.edu/content/connecting-hpc-resources

- ➔ SSH is the traditional first point of access to MSI resources
- ➔ Access **agate mesabi** or **mangi**
- ➔ Uses ssh program available on most personal computers

These “login nodes” are shared by many MSI users. They are NOT for heavy computational tasks. Appropriate uses include:

- ✓ Browsing and editing files
- ✓ Submitting jobs
- ✓ Querying job status and other informational commands
- ✓ Browsing software modules
- ✓ *Light* testing or software compilation



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Interactive Batch with 'srun'

srun <resource requests> --pty bash

See: https://www.msi.umn.edu/content/interactive-queue-use-srun

- Dedicated compute resources via the scheduler
- Command line terminal running on the cluster
  - similar to a SSH session
- Supports all usual Slurm options and commands
- Best used with interactive partitions
  - have priority access for small interactive job requests
- Job terminates when shell exits or connection broken

Example:

```
srun -N 1 --ntasks-per-node=4  --mem-per-cpu=1gb -t 1:00:00 -p interactive --pty bash
```


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Jupyter Notebooks Portal

https://notebooks.msi.umn.edu

See:
https://www.msi.umn.edu/support/faq/how-do-i-get-started-jupyter-notebooks

- JupyterLab web-based computational workspace
- Jupyter Notebook document-oriented computing
- Python and R support provided, users can install additional languages/environments
- Integrated terminal, file editing and browsing
- Runs via scheduler, multiple resource options available
- Session persists until time expires or manually shut down

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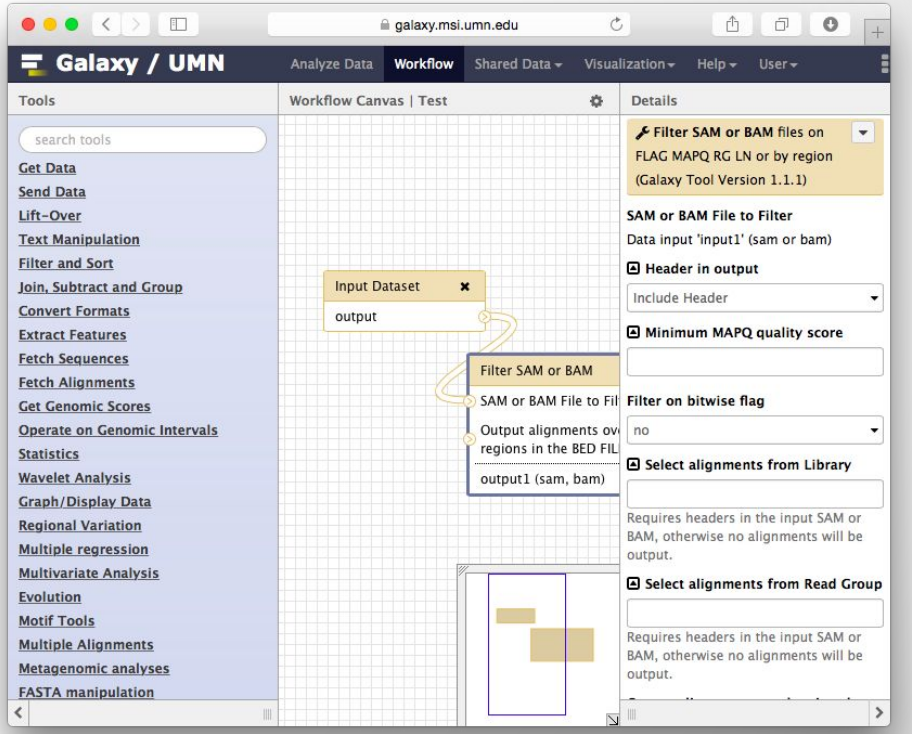
Web Portals: Galaxy

http://galaxy.msi.umn.edu

Galaxy is a web-based workflow manager, principally for bioinformatics/'omics research

- ➔ Compose data analysis workflows in a unified data flow view
- ➔ Workflows execute when requested on MSI compute clusters
- ➔ Wide variety of bioinformatics and 'omics applications available as tools

See https://www.msi.umn.edu/content/galaxy for additional details, especially regarding linking data into Galaxy



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Need Windows?

MSI no longer provides Windows application servers.

Select HPC applications that require Windows are available through partnership with OIT via CITRIX

See: www.msi.umn.edu/support/faq/how-do-i-connect-citrix-windows-virtual-machine for access to Apps.umn.edu

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Hands-On: Getting Connected

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Pre-requisites to connect

Campus VPN

https://it.umn.edu/services-technologies/virtual-private-network-vpn

- ➔ MSI services are only available to on-campus network addresses
- ➔ Especially during the pandemic, many users are working off-campus
- ➔ VPN clients and instructions are available from OIT for most operating systems and mobile devices

DUO Authentication

https://it.umn.edu/services-technologies/self-help-guides/duo-set-use-duo-security

- ➔ DUO 2-factor authentication is required for most MSI services
- ➔ DUO is also required to connect to the campus VPN

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Sidebar: Windows SSH and File Transfer

Current Windows 10+ computers will have ssh/scp available from the Windows terminal.

For users who desire a graphical ssh or file transfer client:
https://winscp.net/eng/downloads.php

Download and install both WinSCP and PuTTY*

*MSI recommends WinSCP and PuTTY for Windows users, but does not offer support for these programs. Contact your local IT department for assistance.

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Choosing a Cluster/Partition

See: https://www.msi.umn.edu/content/choosing-job-partition

- Long running jobs and batch jobs run on Agate/Mesabi/Mangi
- MSI compute clusters are heterogeneous (e.g., up to 1TB Memory, GPUs, SSDs, etc.)
  - **Think**: match your needs to available configurations
  - **Do**: reserve the (CPU/RAM/GPUs/etc) that you need
  - **Avoid**: reserving much more (waste, long queue times) **or** less than required (job doesn't finish before walltime expires)

For interactive use, begin with the **interactive** partition and experiment from there.

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Interactive Services
OnDemand

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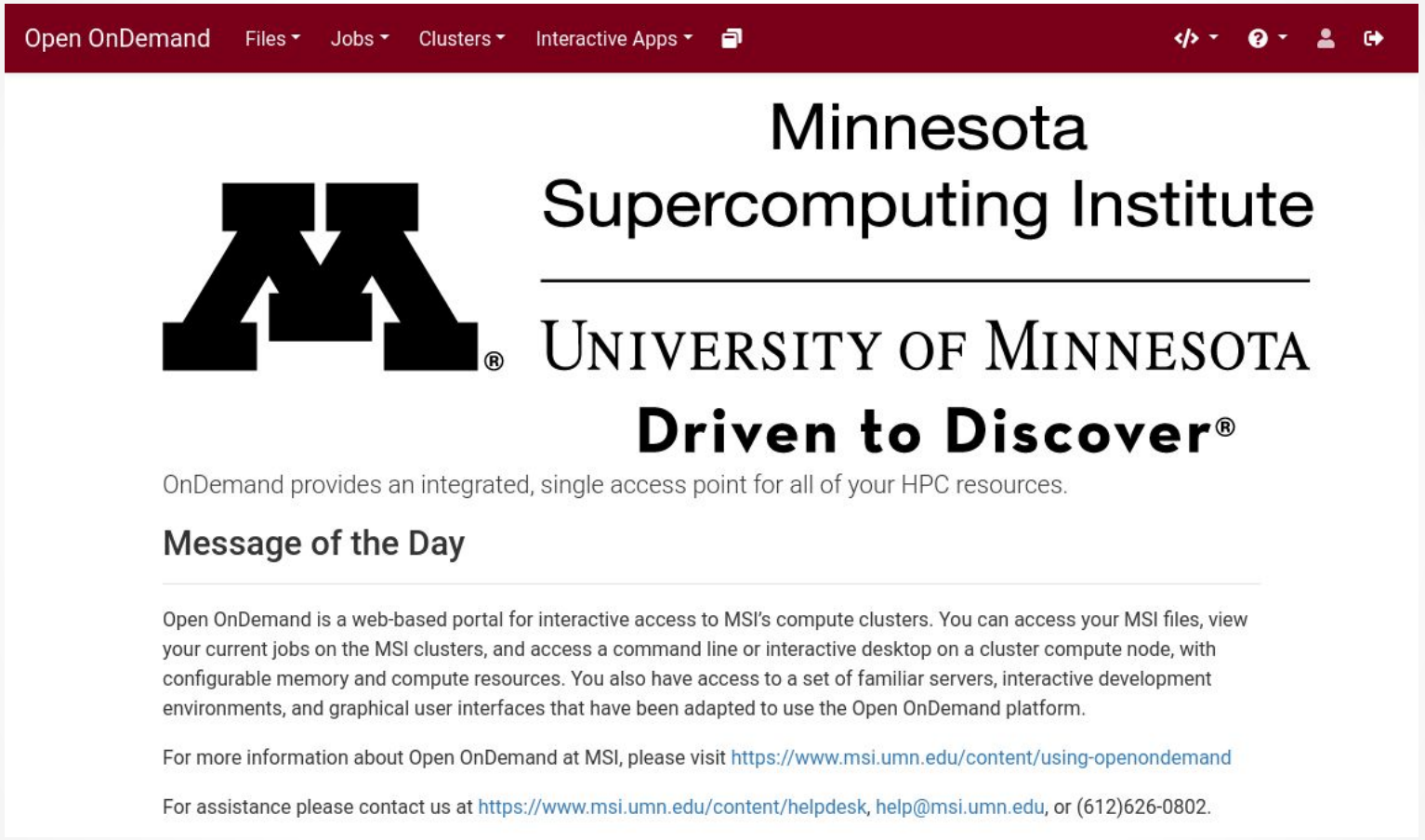
OnDemand Walkthrough



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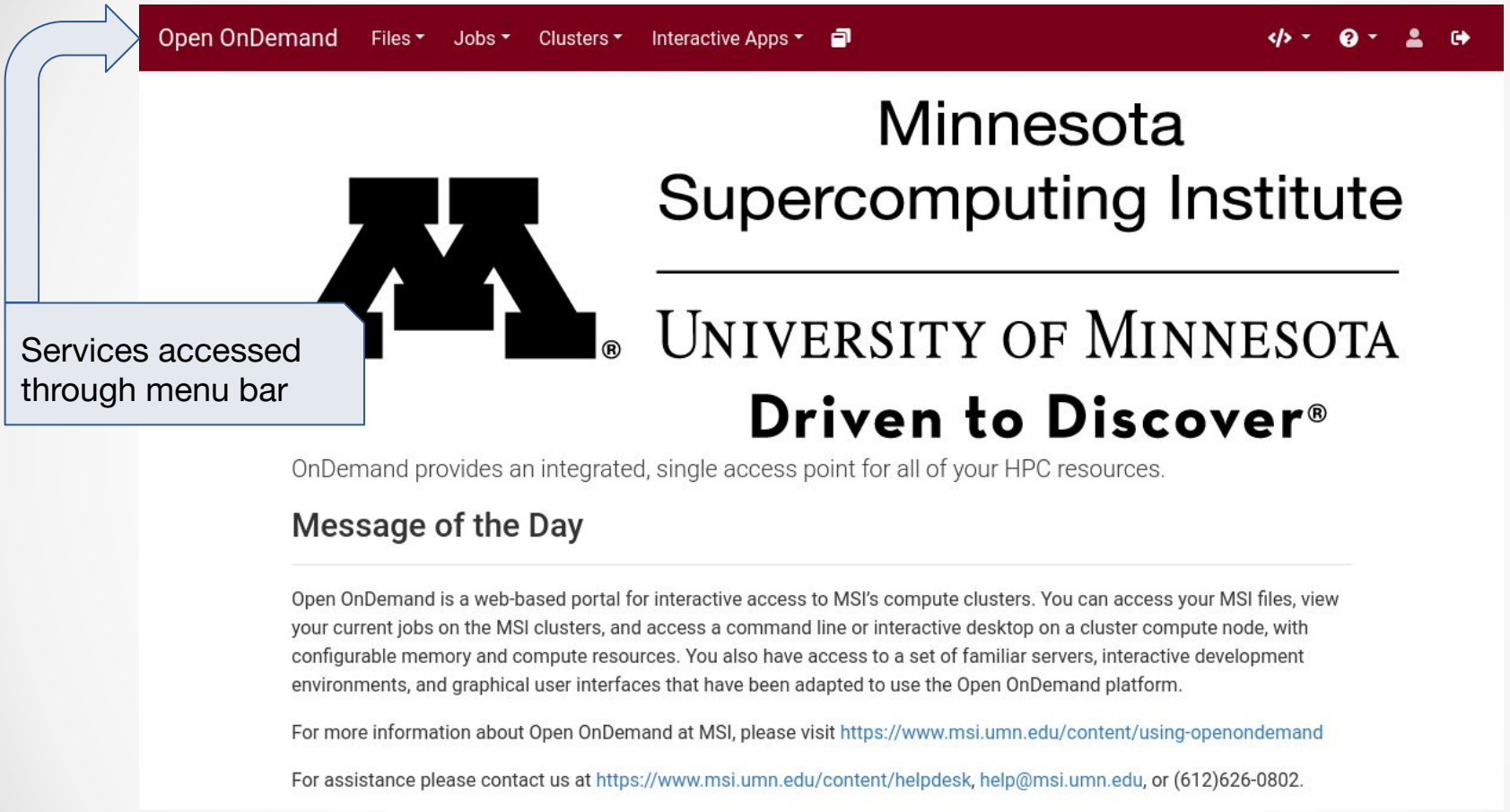
OnDemand Walkthrough



Services accessed through menu bar

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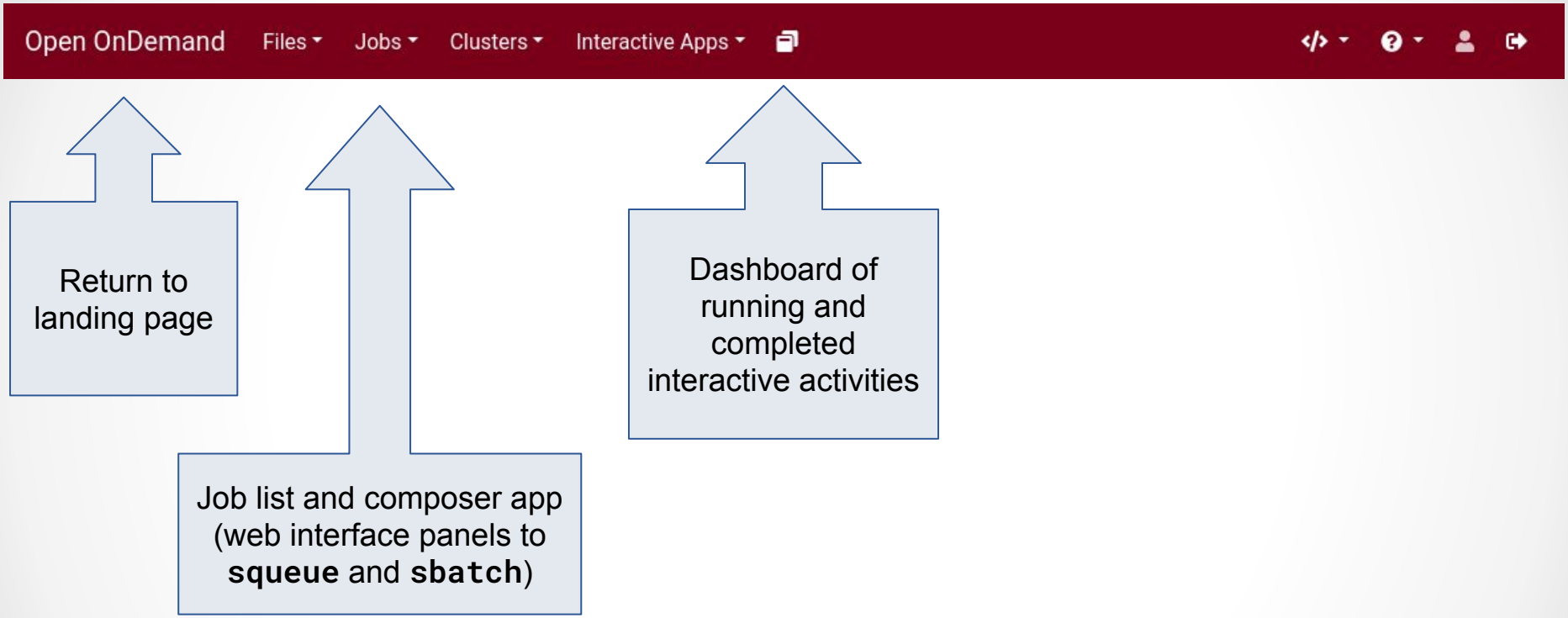
OnDemand Walkthrough



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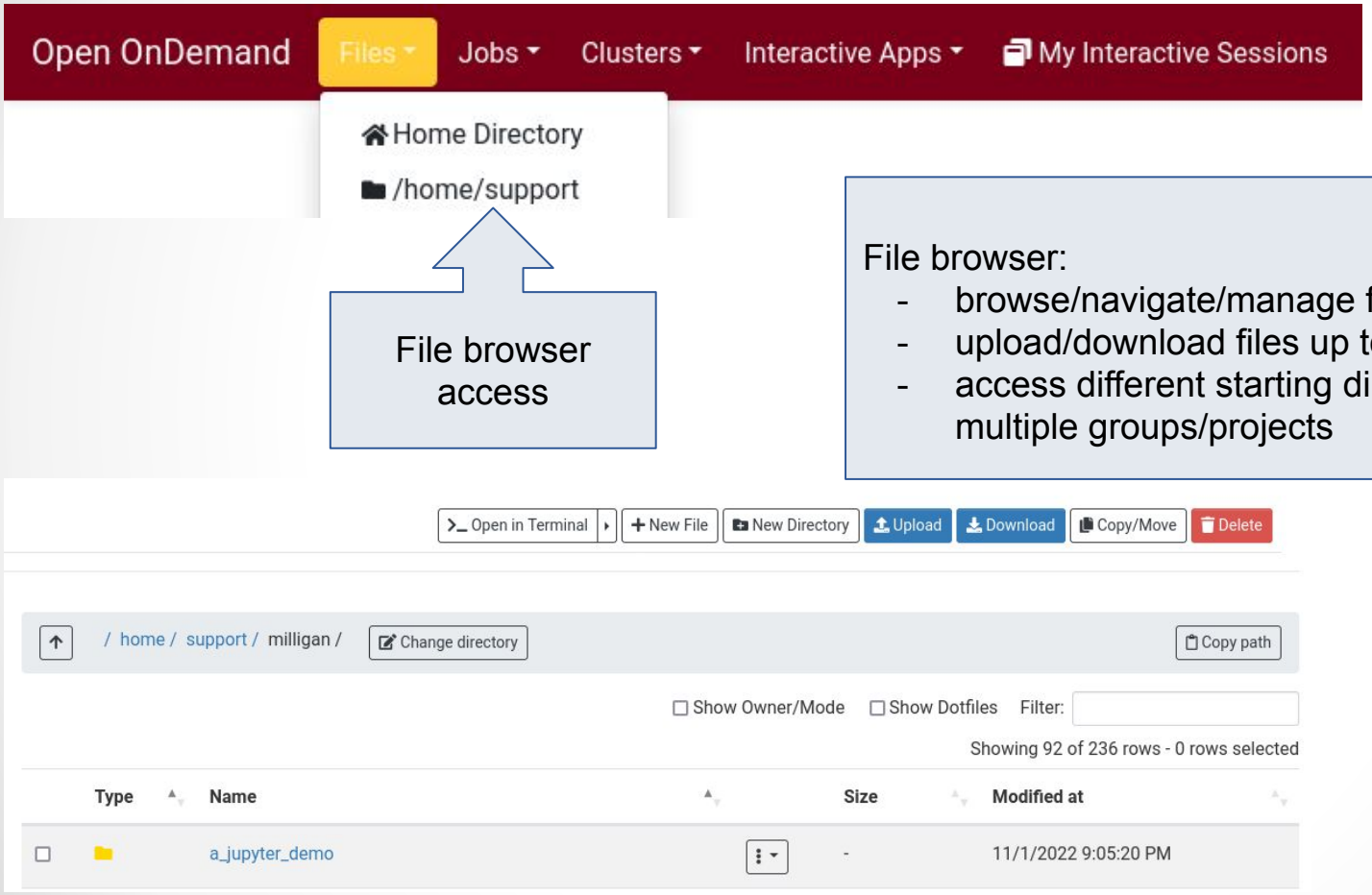
OnDemand Walkthrough



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OnDemand Walkthrough

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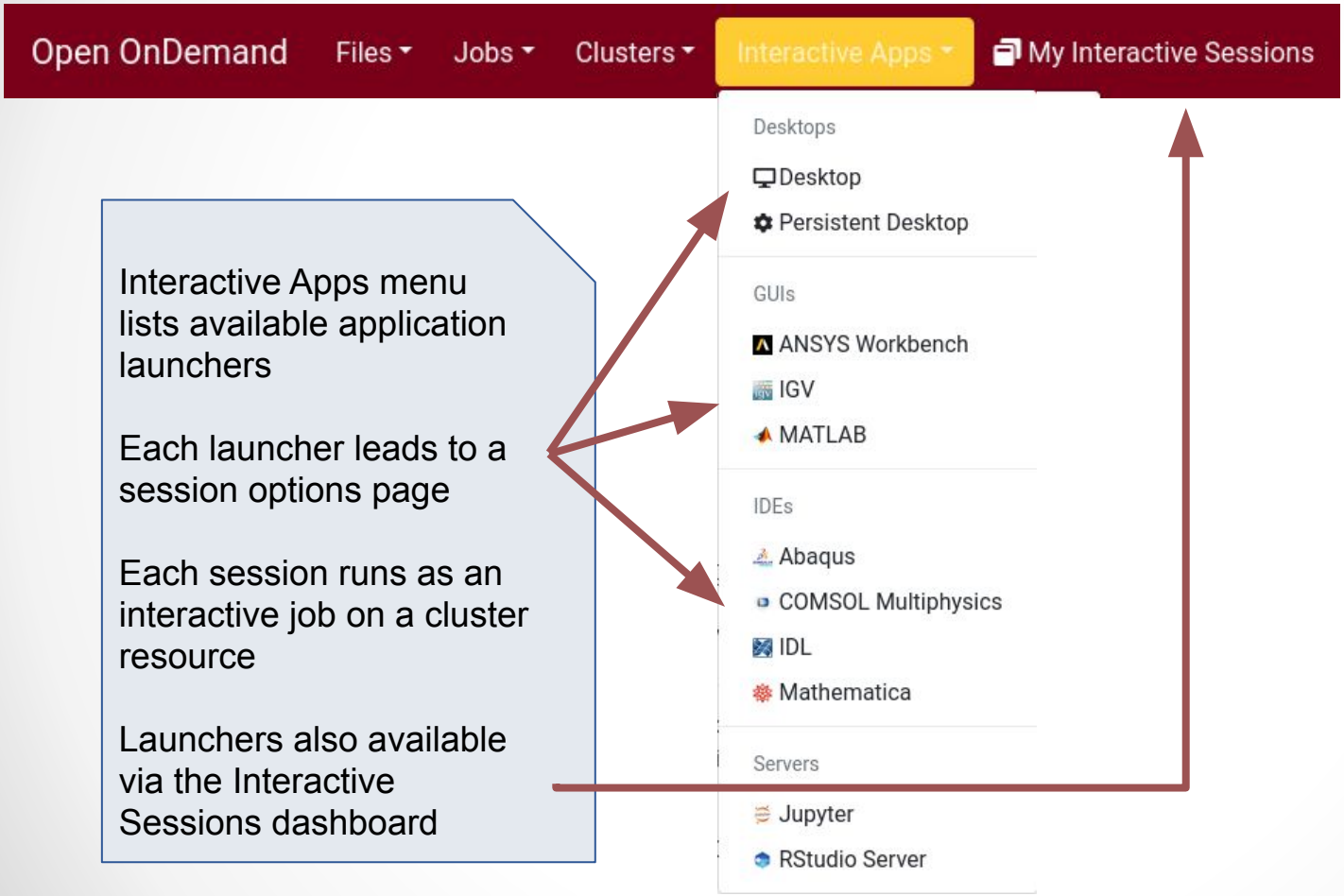
OnDemand Walkthrough



Interactive Apps menu lists available application launchers

Each launcher leads to a session options page

Each session runs as an interactive job on a cluster resource

Launchers also available via the Interactive Sessions dashboard

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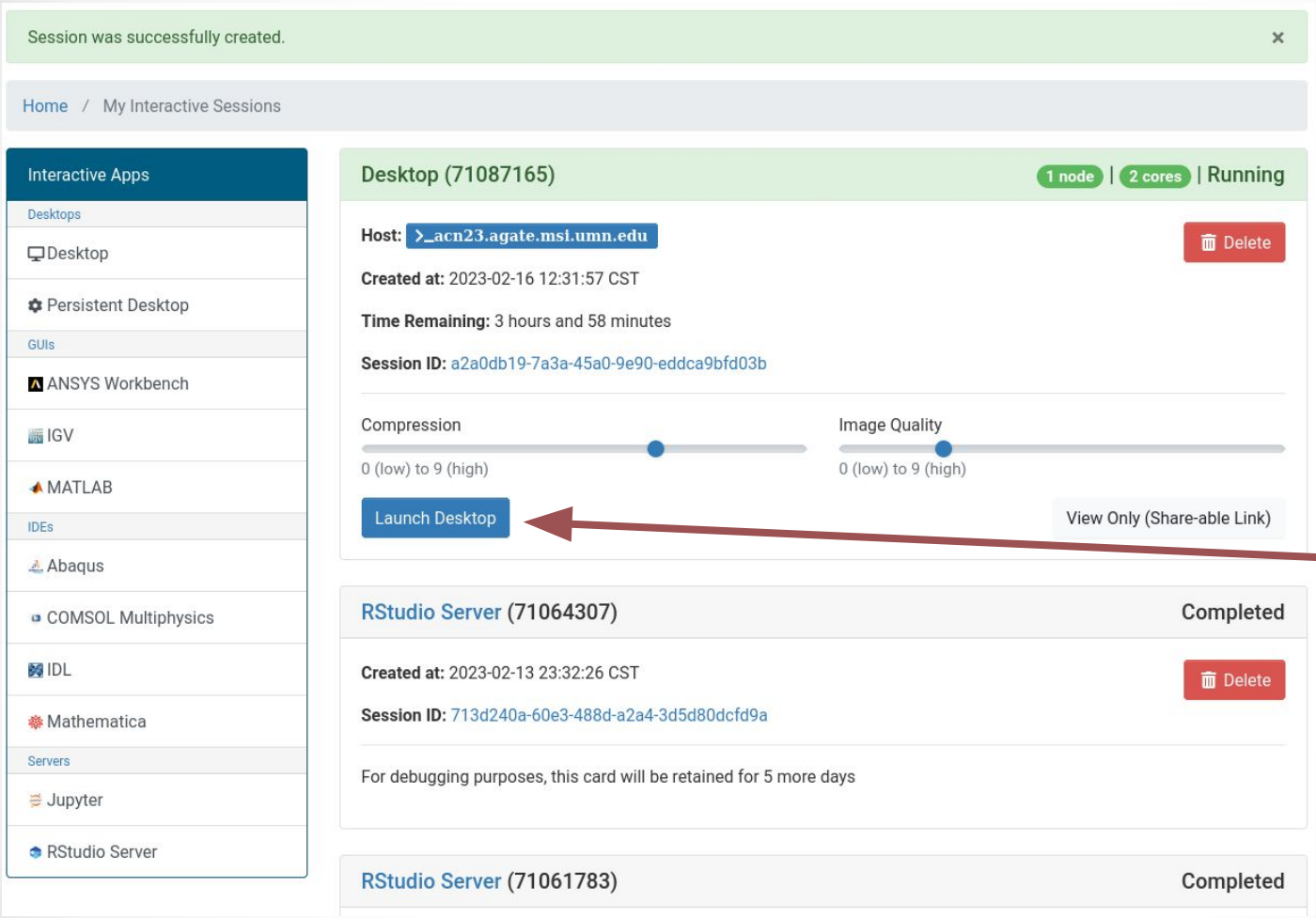
OnDemand Walkthrough



My Interactive Sessions

List job status for interactive sessions: queued, running, finished

Launch into a running session (usually opens new browser tab)

Access full menu of interactive launchers

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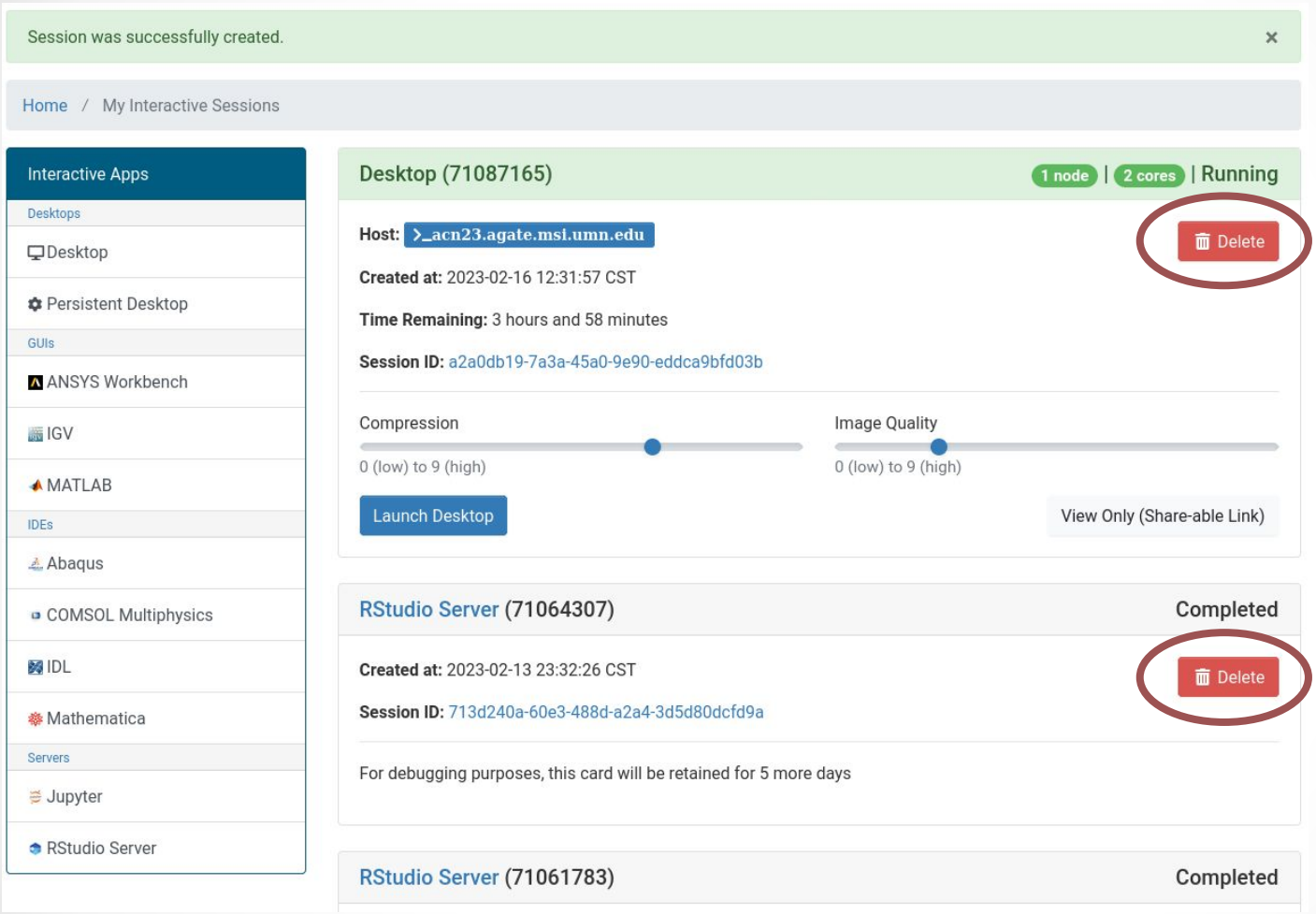
OnDemand Walkthrough



My Interactive Sessions

Delete a running or queued session to cancel the job and release compute resources early

Deleting a completed job removes it from this dashboard; no other effect

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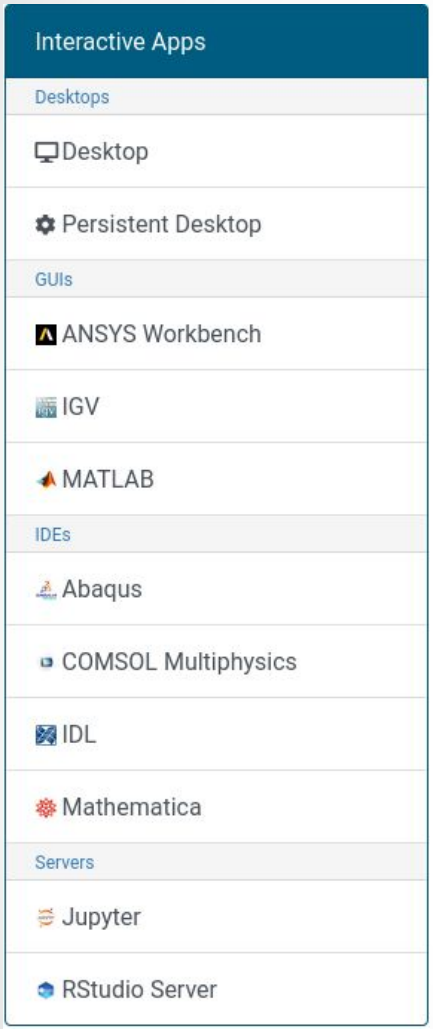
OnDemand Walkthrough



Remote desktop sessions
VNC embedded in a web browser

Runs on compute node in selected cluster resource

These launchers start a remote desktop session and launch corresponding application

Jupyter and RStudio servers run on compute node

Web interface proxied through OnDemand

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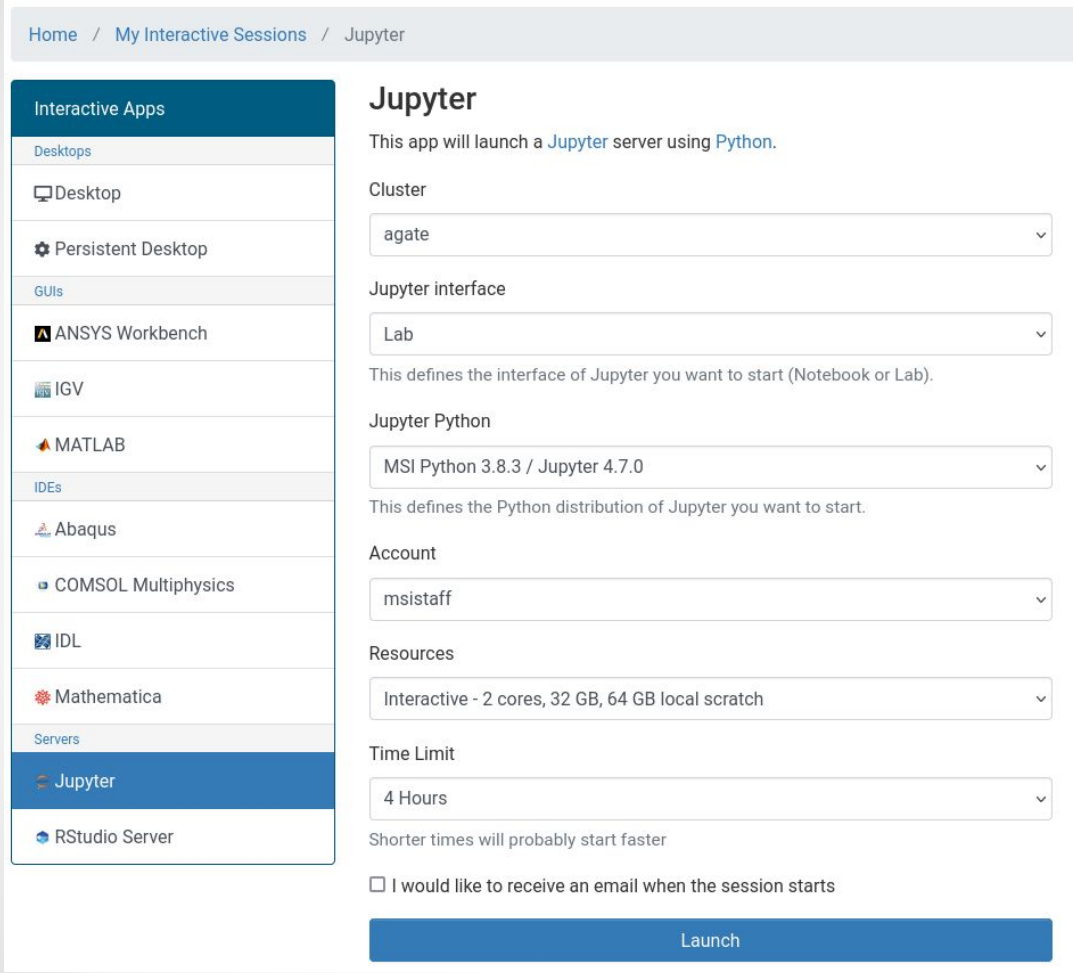
OnDemand Walkthrough



Example launcher:
Jupyter server

Options to customize most aspects of the interactive job

- cluster / partition
- group (if multiple available)
- resource requests
- launcher-specific parameters (e.g. Python environment for Jupyter servers)

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OnDemand Walkthrough

Session cleanup

OnDemand sessions run as scheduled jobs: cancel jobs or use desktop “logout” to end jobs and release resources early, or allow them to close automatically when walltime expires

Logging out from this page clears browser login but otherwise has no effect on active OnDemand sessions

Rarely may need to use “restart server” option to recover from failures

Logout and server restart options

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Interactive Jobs with `srun`

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Selecting Resources

- SSH to any cluster headnode:
  - **`ssh <username>@agate.msi.umn.edu`** or
  - **`ssh <username>@mesabi.msi.umn.edu`** or
  - Launch interactive terminal in OnDemand
- Queue an Interactive job on the cluster:
  - **`srun <job options> --pty bash`**

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Selecting Resources

Options to srun specify job requirements:

- **`srun`** [options]
  - **`--time=8:00:00`** job can run for up to 8 hours
  - **`-N 1 --cpus-per-task=4`** job requests 4 CPUs on one node
  - **`--mem=2500m`** job requests 2500 MB (2.5GB) of RAM
  - **`-p interactive`**
  - **`--pty bash`** job must specify shell program to run
- Enable graphics via X-tunneling (**`--x11`**)
  - not available in web terminals (OnDemand, Jupyter, etc)

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Selecting Resources

Example - basic interactive session with 4 CPU cores, 8 GB RAM, 4 hours runtime:

```
srun -N 1 --ntasks-per-node=4 --mem-per-cpu=1gb -t 1:00:00 -p interactive --pty bash
```

Example - interactive session for machine learning with 1 A40 GPU, 12 CPU cores, 1 hour runtime:

```
srun -n 12 -t 1:00:00 -p interactive-gpu --gres=gpu:a40:1 --pty bash
```


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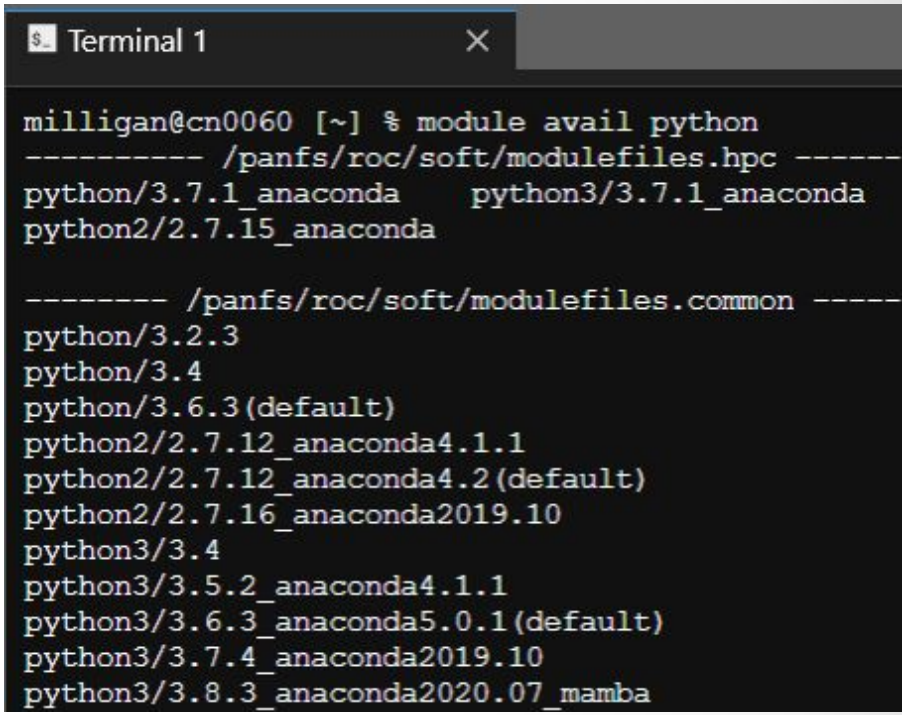
Software Modules

See: https://www.msi.umn.edu/content/accessing-software-resources

- See all modules available
  - `module avail`
- Load a module (adds commands to your shell)
  - `module load python3`
- Run the software from the module
  - `ipython`



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Optional: SSH Keys

- SSH keys allow terminal logins without typing a password repeatedly
- Some applications may automatically make SSH connections and may require SSH keys
- See: www.msi.umn.edu/support/faq/how-do-i-setup-ssh-keys

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Clean up your session

- Delete the session (choose one)
  - Exit out of all connections
  - scancel <job ID>
- What happens on disconnect/delete?
  - All computation stops
- How to resume?
  - Start from zero; or load intermediate files (if you created them)

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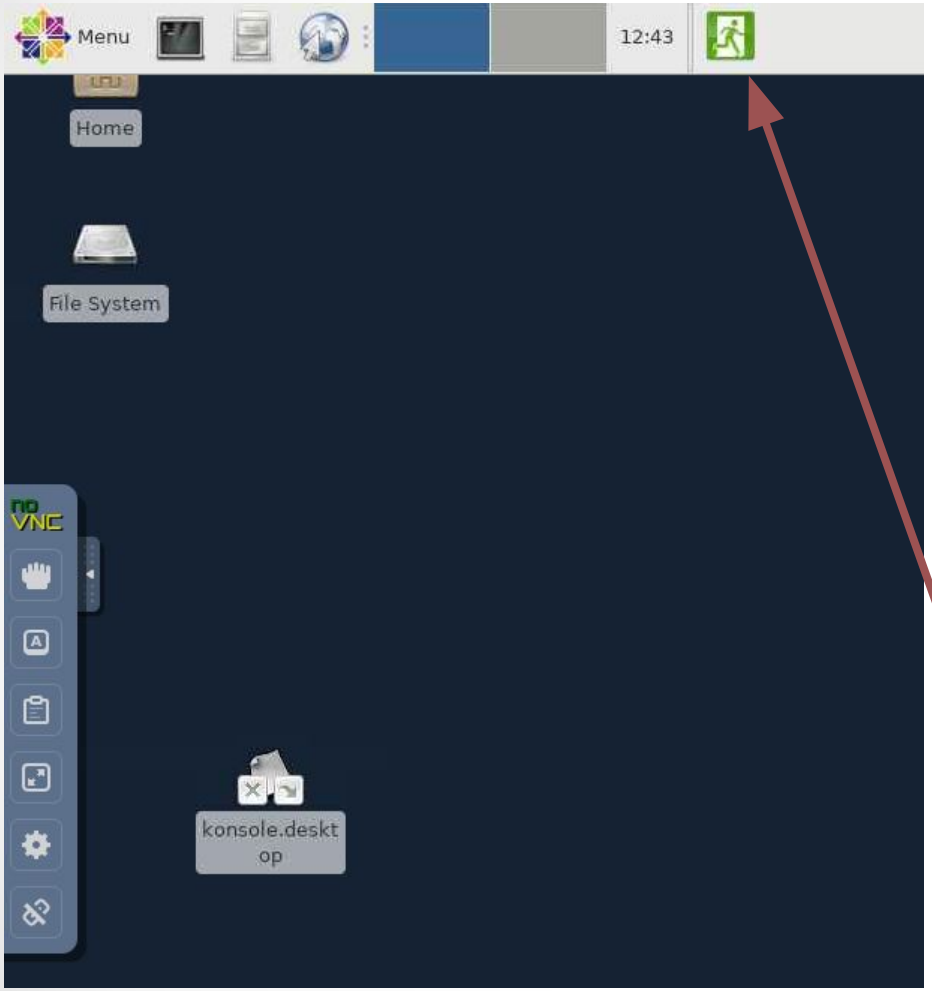
Interactive Linux Desktops



Interactive desktop: noVNC session proxied through OnDemand server

Graphical fidelity will suffer on low-bandwidth connections but quality can be adjusted to maintain usability

Good connections allow graphically intensive apps, GPU accelerated graphics available on GPU nodes

Session persists until logged out on desktop - don't forget to log out to release resources when done!

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Session Clean-up and Resume

- What is lost when the connection drops?
  - Instance: if not expired, reconnect to the same Instance
  - Data: no loss
- What if you Logout?
  - Instance: Terminated; Reconnect and start fresh
  - Data: Scratch data is deleted periodically* (clean up after yourself to be sure); No loss for data in group home
- How do you reconnect?
  - Login again through OnDemand Interactive Sessions dashboard

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Hands-On: Interactive Development and Data Interrogation with Jupyter

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Start your Jupyter Session

- Visit notebooks.msi.umn.edu
- Select the default interactive job
- There will be a short wait while the background job starts running
- When ready, the JupyterLab workspace will load in your web browser window

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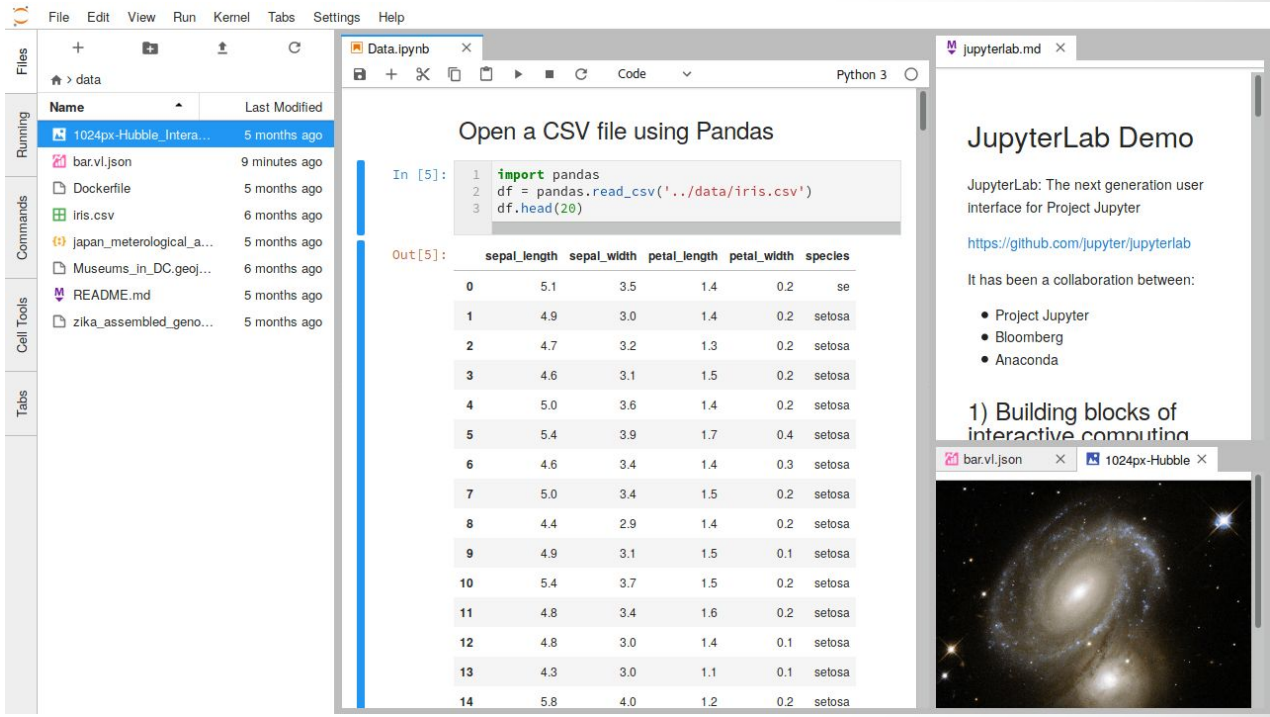
JupyterLab Workspace

See: https://jupyterlab.readthedocs.io/en/stable/user/interface.html

- Rich tabbed multi-document workspace
- File navigation able to access home and group directories
- Reproducible, sharable computational stories in Jupyter Notebooks
- View and edit text and other files directly in JupyterLab
- Command line terminal available



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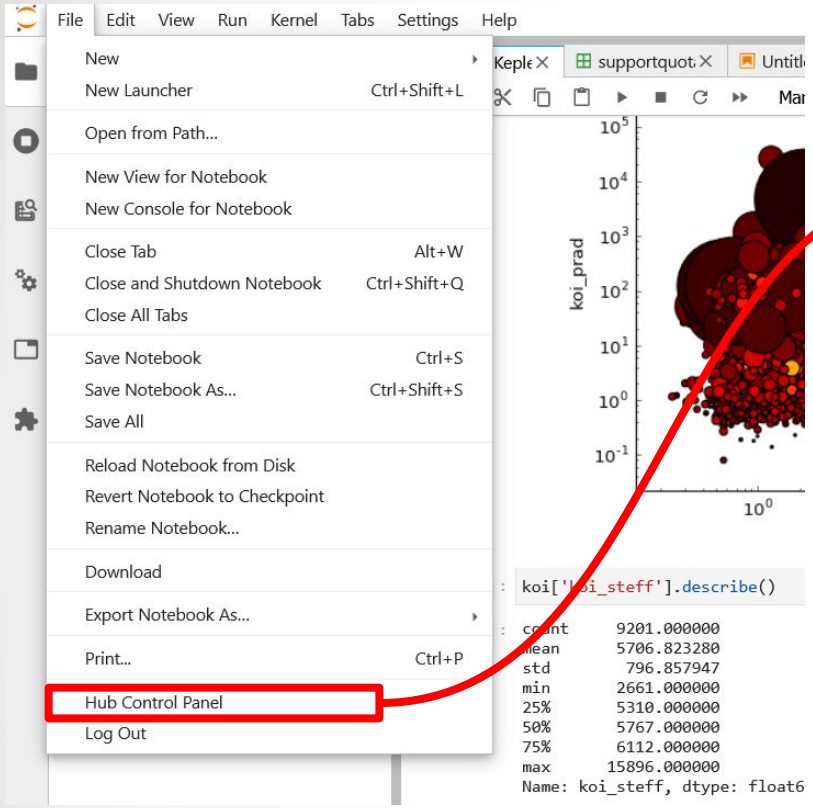
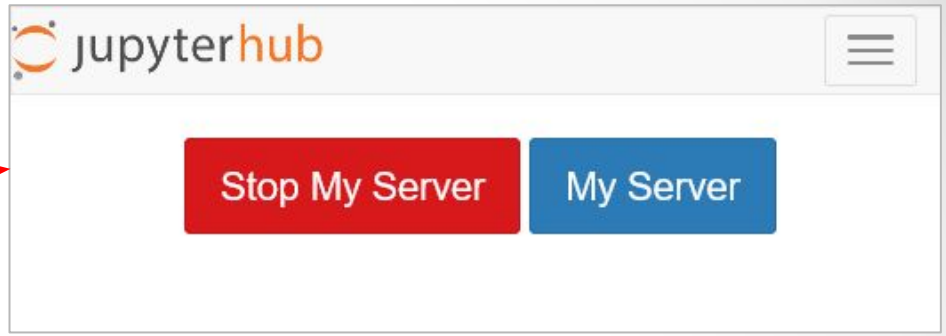
Jupyter Cleanup





- Jupyter sessions persist (for 4 or 12 hours) even if you disconnect or log out
- You can disconnect and reconnect as many times as you want or from different locations
- To terminate a session and stop using resources, access the Hub Control Panel and select Stop My Server

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Additional Documentation

- Overview of IPython's architecture for parallel and distributed computing.
- Detailed discussion of IPython cluster controller and engines.
- Discussion of IPython magic commands
- Official IPython documentation

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Questions?

These slides and the hands-on guide will be posted to http://msi.umn.edu (see the "MSI Tutorials" section)

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