

Rivanna is the university's primary resource for high-performance computing. It provides a platform for computationally-intensive research across disciplines.

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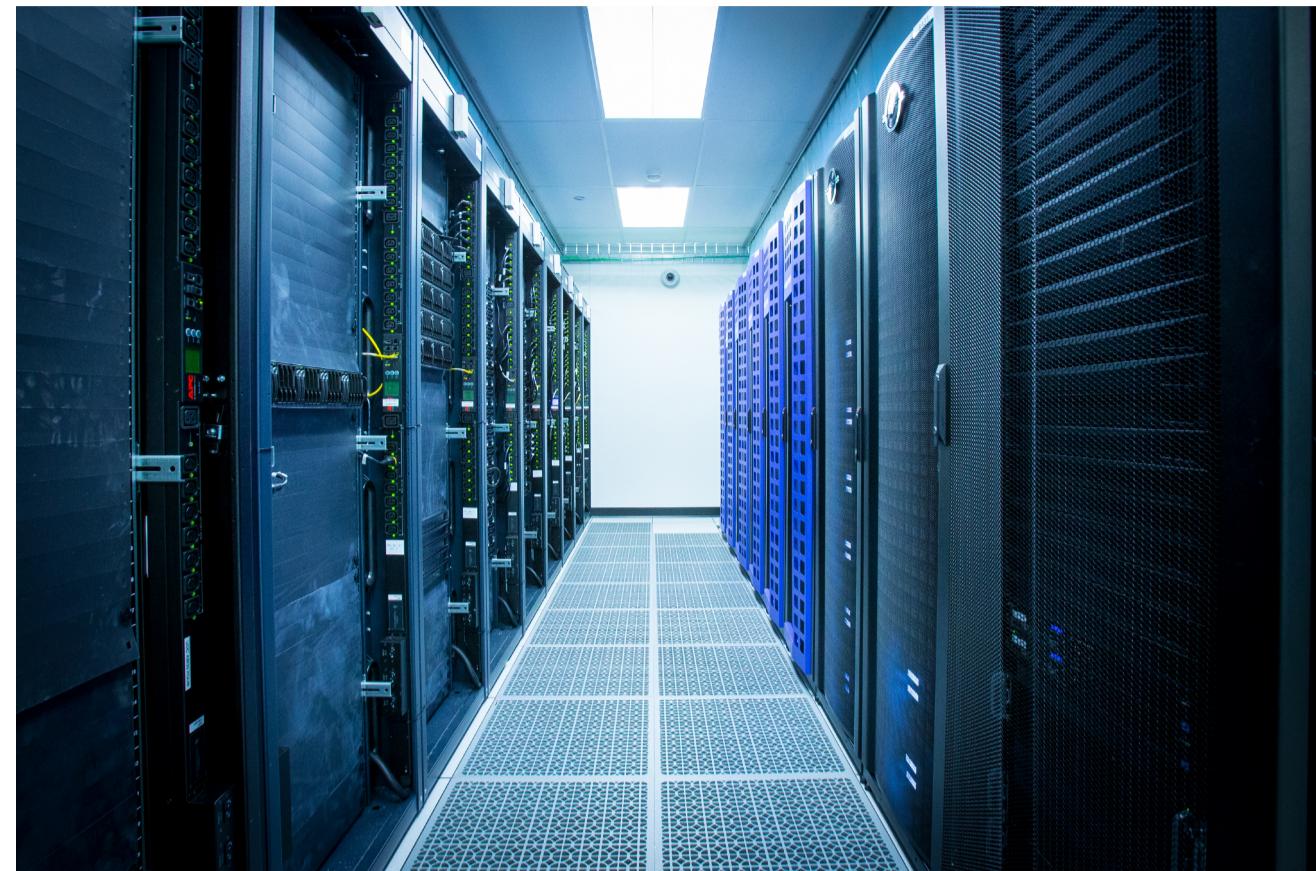
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The Rivanna cluster

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- Node

- A *node* is the basic building block of a cluster.

- Nodes are a type of computer called a *server*.

- They generally have more power than a typical computer.
 - They may have specialty hardware like graphical processing units.

- Two types of nodes

- **Head Node** – a server used for logging in and submitting jobs.
 - **Compute Node** – a server that carries out the computational work.

- Core – an individual processor on a computer

- Rivanna's nodes have many cores (typically 40 each)

- Memory

- The random-access memory on a node

- Storage

- Disk storage visible from a node

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Time on Rivanna is *allocated*.

- An allocation refers to a block of CPU time that you can use to run your computations.
- Only faculty, postdocs, and research staff may request an allocation.
 - Students must be sponsored by a faculty or research staff.
 - All individuals on a given allocation share the service units.
- Allocations may be requested at
<https://www.rc.virginia.edu/userinfo/rivanna/allocations/>
- Allocations are measured in service units (SUs), where **1 SU = 1 core-hour** in most cases. Nodes equipped with GPUs may charge more than one SU per core-hour.

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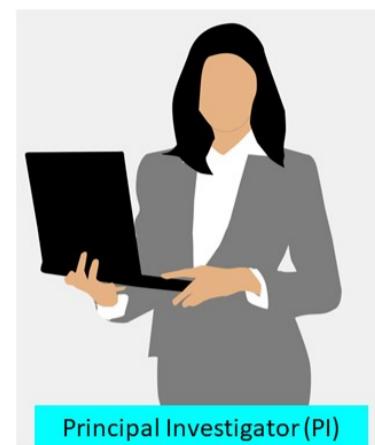
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Login Accounts

- Allocations and Groups
 - An allocation is associated with a *group*. Currently this is a [MyGroups](#) group.
 - Members (but not administrators) of the allocation group automatically receive an account on Rivanna.
 - RC staff do not manage allocation groups. The PI is responsible for adding and removing group members.
 - The PI may designate administrators and delegate the task of managing the group to them.

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System Specifications

Currently the Rivanna supercomputer has 603 nodes with over 20476 cores and 8PB of various storage.

Several queues (or “partitions”) are available to users for different types of jobs. One queue is restricted to single-node (serial or threaded) jobs; another for multi-node parallel programs, and others are for access to specialty hardware such as large-memory nodes or nodes offering GPUs.

More information on queueing policies and hardware configurations can be found on our [website](#).

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Storage

Rivanna users can access free storage for active work. Research groups that need more permanent storage, or wish to share storage space, can also lease storage.

No-Cost Storage

Each user has access to a *home directory* and a *scratch directory*.

Home Directory

When you log in, you will be in your home directory, e.g. /home/mst3k. Each home directory on Rivanna has 50GB of storage capacity. The home directory is for individual use and is not shareable with other users.

Scratch Directory

You have access to 10 TB of **temporary** storage. It is located in a subdirectory under /scratch, followed by your userID, e.g., /scratch/mst3k

The /scratch directory is for individual use and is not shareable with other users.



/scratch is **NOT** permanent storage and files that have not been accessed for more than 90 days will be marked for deletion.

Leased Storage

We offer two tiers of leased storage. For rates and offerings see our [website](#).

Research Standard Storage

Standard storage is inexpensive but is not backed up, and access from Rivanna is slow.

Research Project Storage

Research project storage provides *snapshots*. Snapshots are not backups, but are a "snapshot" of the files over a time interval in the past, currently one week.

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Connecting and Logging On To Rivanna

- There are three ways to connect to Rivanna:
 - Open OnDemand, a graphical user interface through a web browser
 - you can examine and manipulate files and submit jobs.
 - you can access applications such as Matlab, Jupyterlab, and R Studio Server.
 - FastX Web, direct access to a desktop for Rivanna
 - ssh (Secure Shell) client, which provides direct access to the command line.
 - For Windows we recommend [MobaXterm](#)

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Open OnDemand

To connect to Open OnDemand, open your web browser and type

<https://rivanna-portal.hpc.virginia.edu>

You will need to authenticate with Netbadge ("Netbadge in")

You can connect to Open OnDemand from off-Grounds locations without a VPN connection.

Remember that Open OnDemand is a Web application. If it freezes on you, click **UVA Open
OnDemand** in the upper left. It will log you out eventually so you may need to log in again. You
also may have to refresh pages to see changes.

It may also open many tabs. It is safe to close them if you aren't using them; just make sure
you first click "Save" for any files you are editing and want to save changes. You can even
close all the tabs and log in again.

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Open OnDemand Dashboard

The Open OnDemand home page is the Dashboard.

OnDemand provides an integrated, single access point for all of your HPC resources.

Message of the Day

2023-08-15 Scratch Directory All data in /oldscratch i.e. /gpfs/gpfs0/scratch will be **permanently removed on October 17, 2023**. Please back up your data. The 90-day purge policy will be implemented for /scratch - files not accessed in 90 days are removed. /scratch is intended as temporary storage for active work. It is not backed up and needs to be purged periodically in order to maintain a stable HPC environment. RC offers several low-cost storage options to researchers; see [here](#).

powered by **OPEN OnDemand** OnDemand version: 2.0.32

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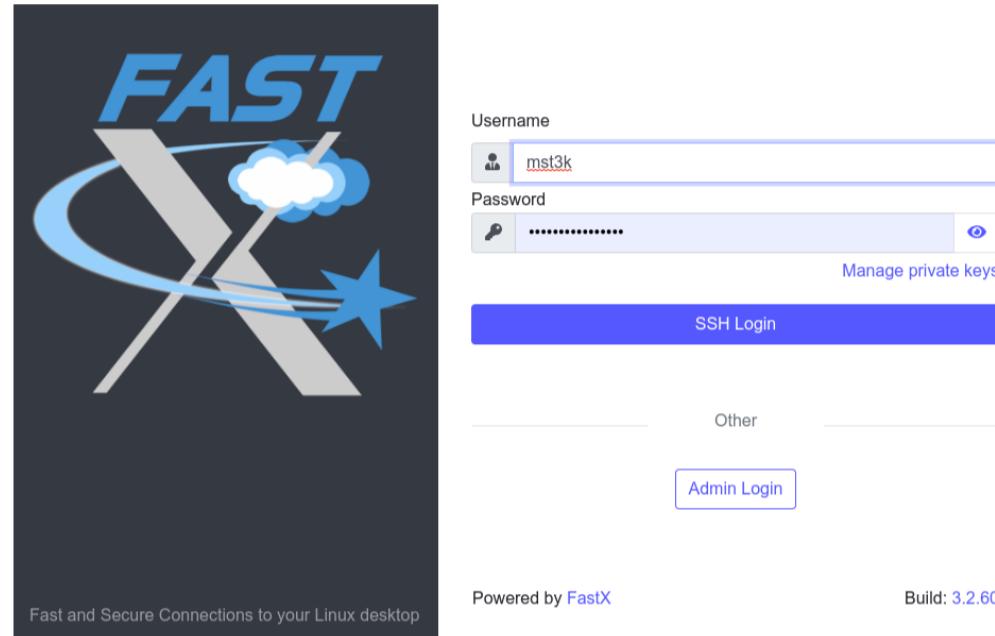
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Connecting with FastX

FastX is a Web-based desktop environment for HPC. It is accessible either through the [Open OnDemand Interactive Apps](#) menu, or directly at <rivanna-desktop.hpc.virginia.edu>.

FastX requires the VPN. If the VPN is not active, the start page *will not load*.

Always use either the OOD link or the <rivanna-desktop> URL. The underlying name of the host may change from time to time.



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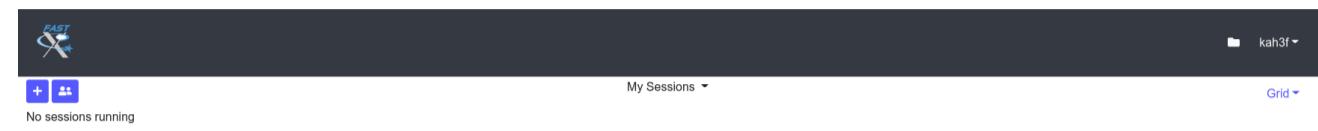
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The FastX Session

FastX starts a session on a Rivanna frontend. A new session is started by clicking the [+](#) button.



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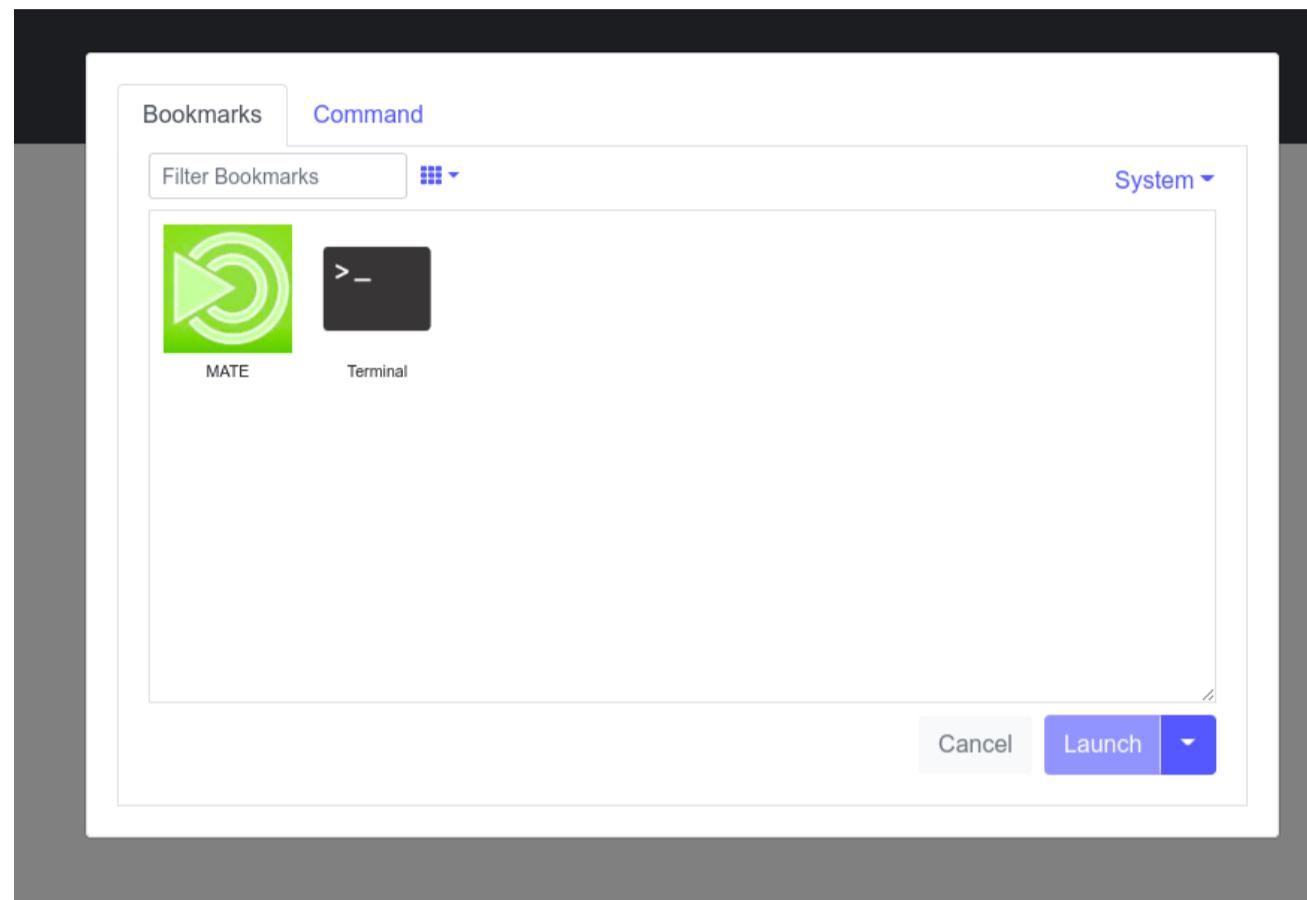
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Most users should chose the MATE session. Click the icon, then click the **Launch** button.



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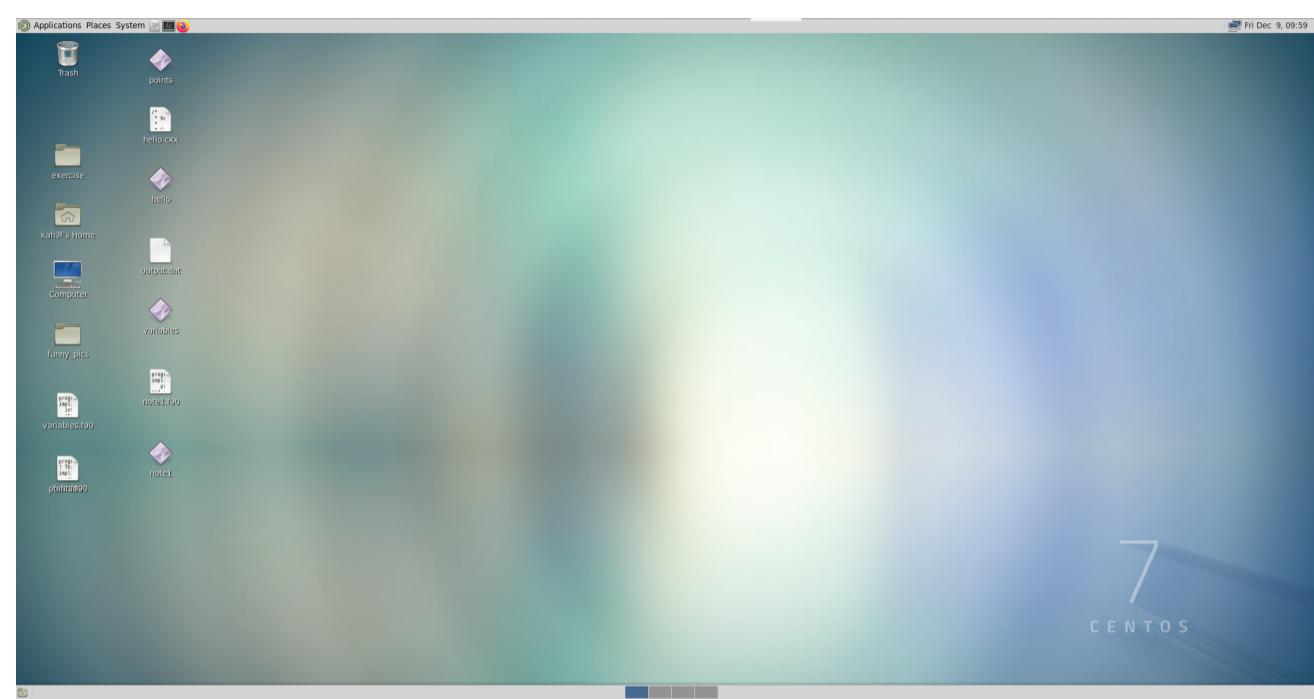
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A MATE desktop looks a little like an older Windows desktop. In the ribbon at the top are [Caja](#), a file manager; a [Terminal](#) application, and the Firefox Web browser.



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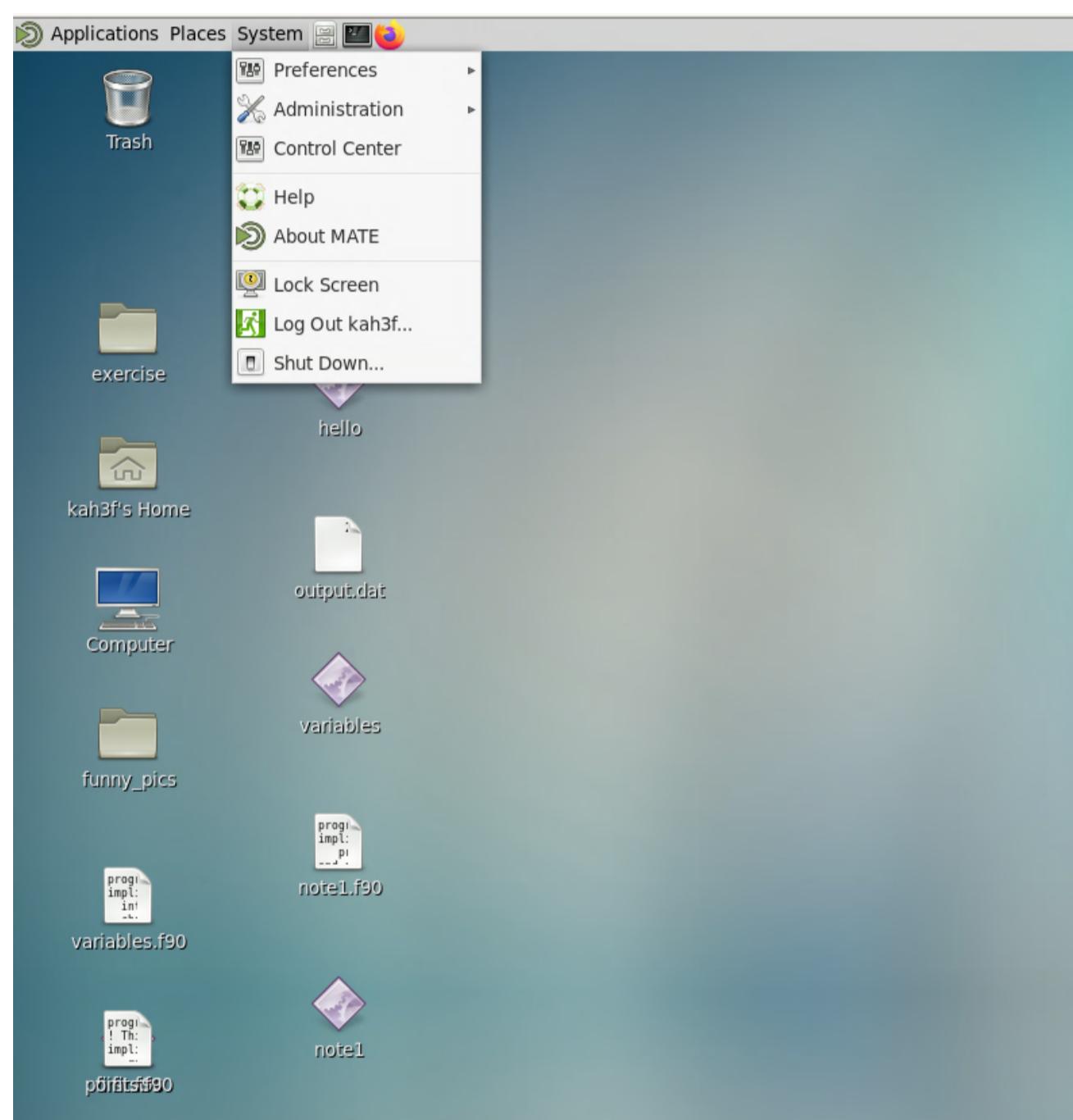


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Logging Out of FastX

If you simply close your session browser tab, FastX *suspends* your session rather than terminates it. It is generally preferable to terminate rather than suspend so you will not accidentally have multiple sessions running.

One way to terminate is to log out. Go to the System menu in the top ribbon and select **Log Out** `mst3k` (with your ID).



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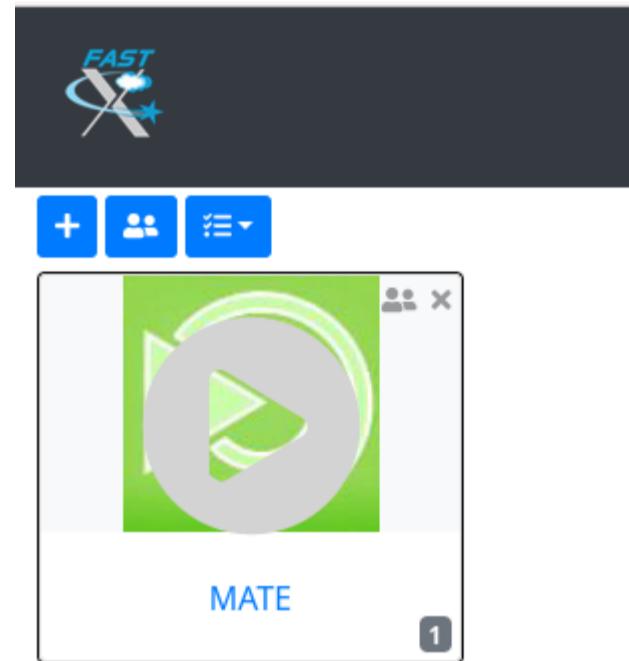
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Terminating or Restarting FastX

You can also terminate – or restart – a session from the My Sessions tab. To terminate, click the **x** in the upper right of the session, or use the menu.

To restart instead of terminating, click the arrow for “run”.



Terminating or restarting a session.

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Interactive Apps with Open OnDemand

Open OnDemand's File Explorer, the FastX Web interface, and various command-line interfaces, can be used to prepare work for the cluster. This includes transferring and editing files, looking at output, and so forth. However, all production work must be run on the compute nodes, not on the frontends.

A large, multi-user system like Rivanna must be managed by some form of *resource manager* to ensure equitable access for all users. Research Computing uses the [Slurm](#) resource manager. Resource managers are also often called *queueing systems*. Users submit *jobs* to the queueing system. A process called a *scheduler* examines the resource requests in each job and assigns a priority. The job then waits in a *queue*, which Slurm calls a *partition*, until the requested resource becomes available. A partition is a set of compute nodes with a particular set of resources and limits. On Rivanna there are partitions for single-node jobs, multiple-node jobs, GPU jobs, and some other dedicated partitions. A list of the different queues and resources are listed below.

Queue Name	Purpose	Max time / job	Max nodes / job	Max cores / job	Max cores /node	Default memory /core	Max memory /node / job	SU Charge Rate
standard	For jobs on a single compute node	7 days	1	37	37	9 GB	750 GB	1
gpu	For jobs that can use general purpose graphical processing units (GPGPUs) (K80 or P100)	3 days	4	32 GPUs	125	6 GB	1953 GB	3
parallel	For large parallel jobs on up to 50 nodes (<= 1850 cores/job)	3 days	50	1500	40	9 GB	375 GB	1
largemem	For memory intensive jobs (<= 45 cores/node)	4 days	2	32	45	60 GB	1464 GB	1
dev	To run jobs that are quick tests of code (<= 2 nodes, 25 cores/node)	1 hour	2	16	25	6 GB	246 GB	0

Queue Information

Open OnDemand offers an easy way to run *interactive* jobs. With an interactive job, you are logged in directly to a compute node and can work as if it were a frontend. Please keep in mind that an interactive job terminates when the time limit you specify expires, unless you explicitly end the session.

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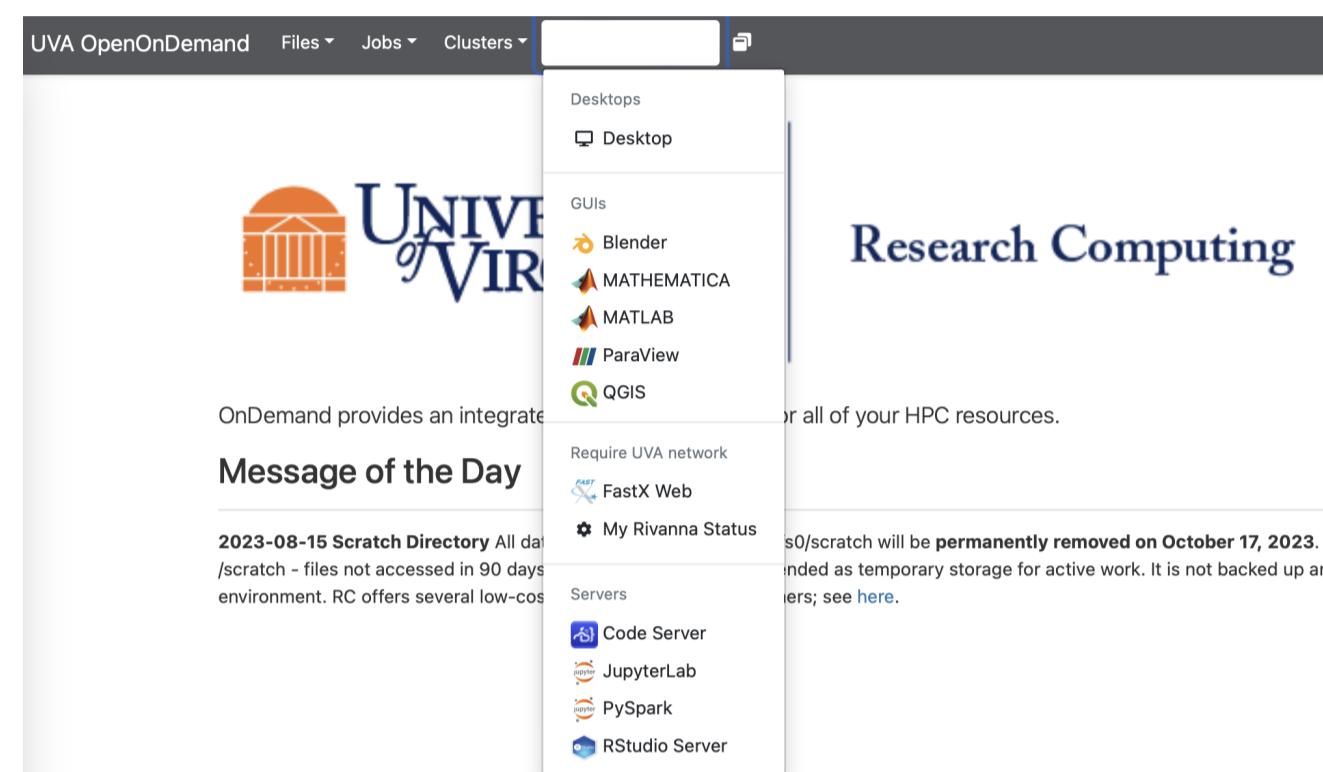
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The OOD Interactive Apps Menu

To submit an interactive job, from the Open OnDemand dashboard click on the menu [Interactive Apps](#) for the dropdown list.

We will focus on JupyterLab, Rstudio Server, and the Desktop for now.



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Interactive JupyterLab Sessions

From the Interactive Apps menu, select JupyterLab.

The Jupyter Web Form gathers information about the computing resources that you need to run your Jupyter Notebook.



After you fill in the form, it will remember settings the next time that you connect to it, so watch out if you wish to change something.

JupyterLab

This app will launch [JupyterLab](#) on the Rivanna cluster.

Rivanna Partition

Standard

- **Dev** - (1 core) For short sessions (1 hour) with no SU charge.
- **Standard** - (1-40 cores) Rivanna node in the standard partition.
- **Instructional** - (1-20 cores) Rivanna node in the instructional partition.
- **GPU** - (1-28 cores) Rivanna node that has NVIDIA GPU.
- **Bii,Bii-gpu** - (1-40 cores) Partition for Biocomplexity Institute and Initiative.
- **Learn More** - [Rivanna Queuing Policies](#)

Number of hours

1

Number of cores

1

Memory Request in GB (maximum 384G)

6

Work Directory

HOME

Allocation (Research or Class MyGroup) - lowercase-only

your_allocation

- [MyGroup](#)

Show Additional Options

No

I would like to receive an email when the session starts

Launch

* The JupyterLab session data for this session can be accessed under the [data root directory](#).

Setting up a job in JupyterLab through OOD

You must choose a partition from the dropdown list. The partition limitations are explained below the dropdown box. Most of the time, you will select the **Standard** partition. If you are running a deep learning model, you will want to choose a **GPU** Partition. If you do not specify a GPU model, your job will be assigned to the first available.

The “Number of hours” is the time your job session will remain active.



If you exceed the requested time limit, your session will be terminated without warning.

The “Allocation” is the name of the allocation that should be charged. Your advisor should have told you what to use. You can be a member of more than one allocation. In that case one of them, not chosen by you, will be the default. It is best to always fill in the name of an allocation, but remember to change it if necessary.

Once you have completed the Webform, click on the [Launch](#) button to submit the request.

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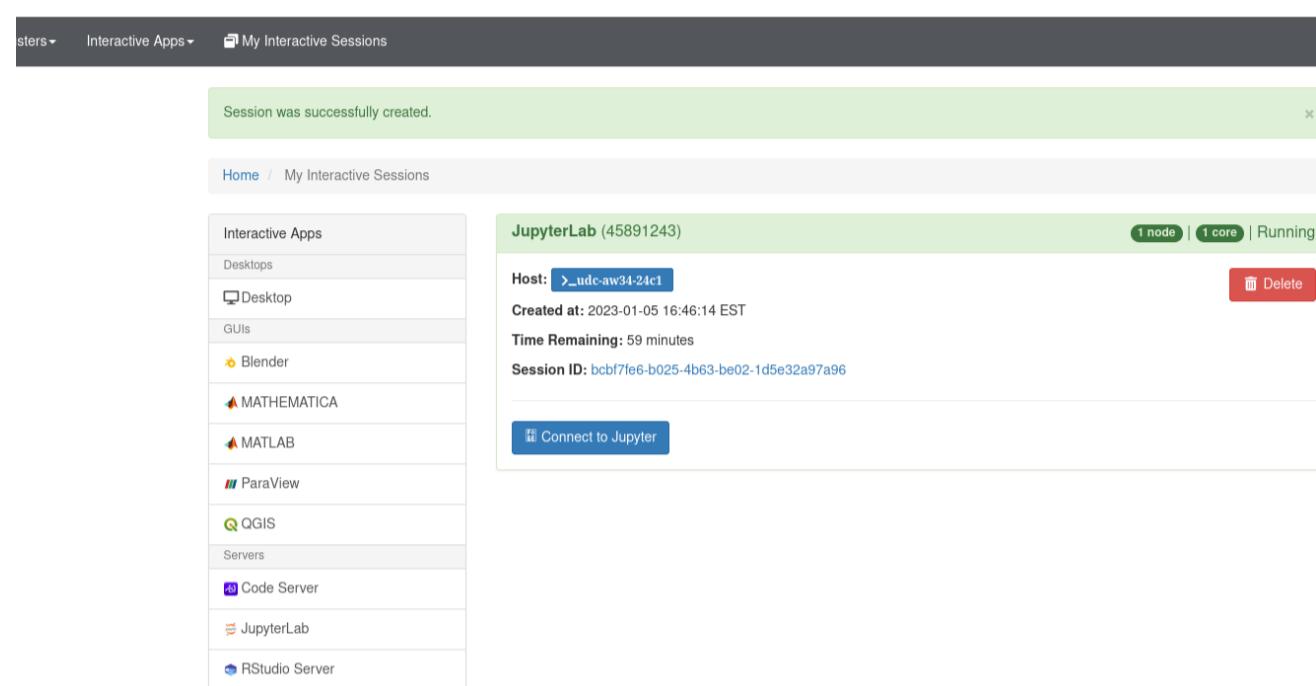


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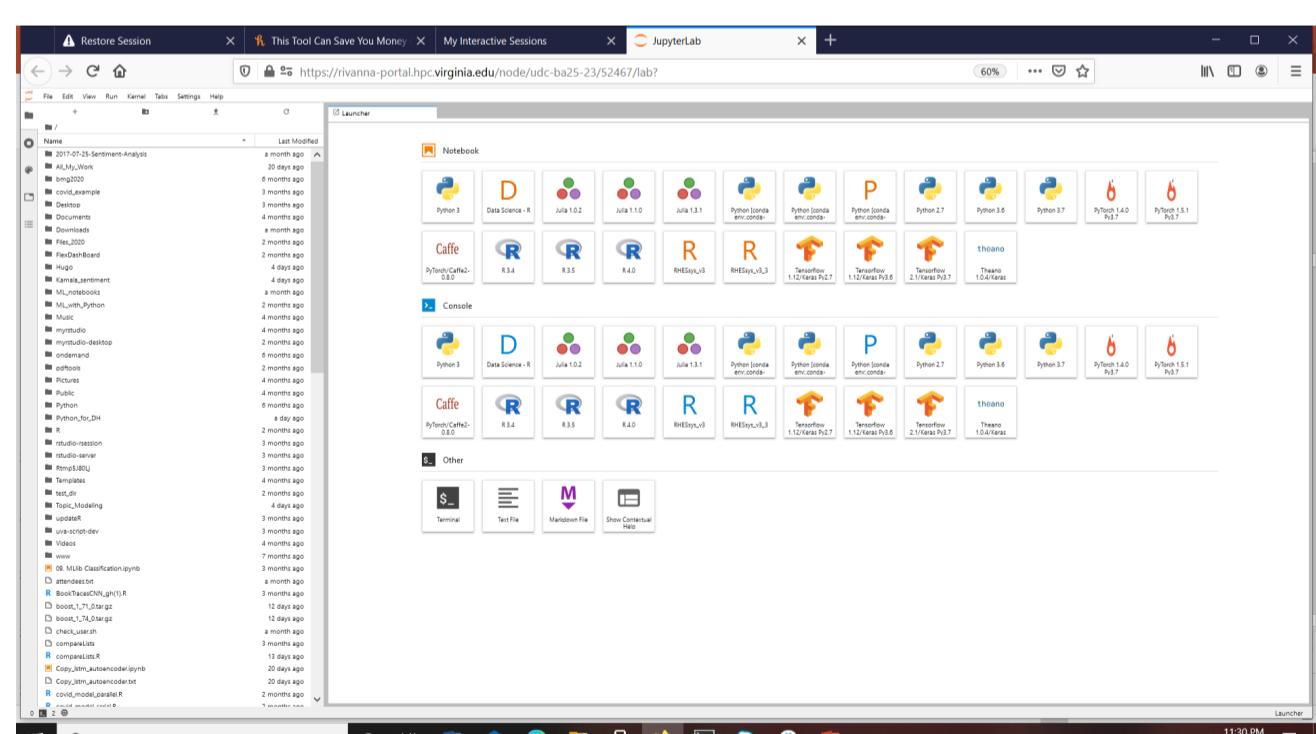
When you submit a request for an interactive app, it will be placed into the partition you specified, where it will wait until resources become available. Requests with higher resource requests (more cores, more memory, more time) may wait longer.

Once the job session begins, the screen will ask you to connect. In our example you will see a **Connect to Jupyter** button appear.



Connecting to a session.

When you connect, you will see your files on the left sidebar and a collection of kernels from which to choose. You may not see all of these “tiles” because some accounts have customized tiles set up.



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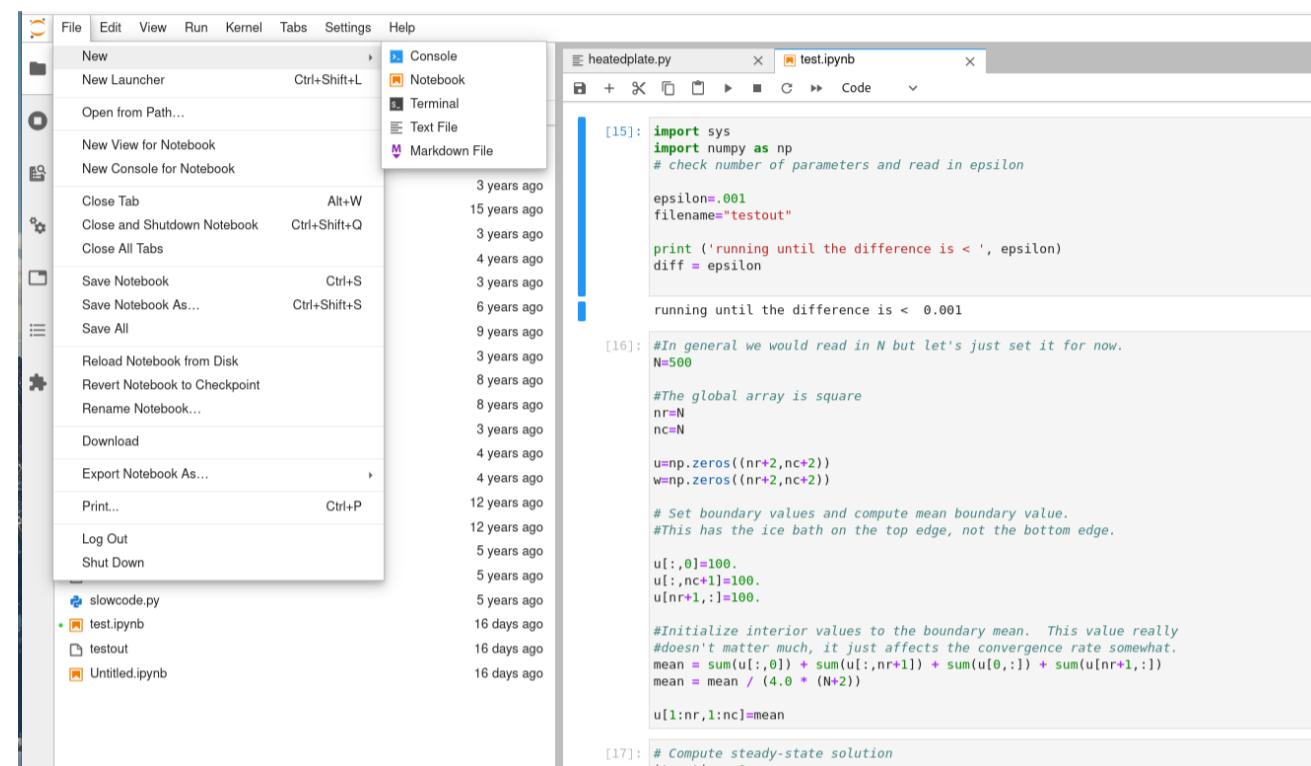
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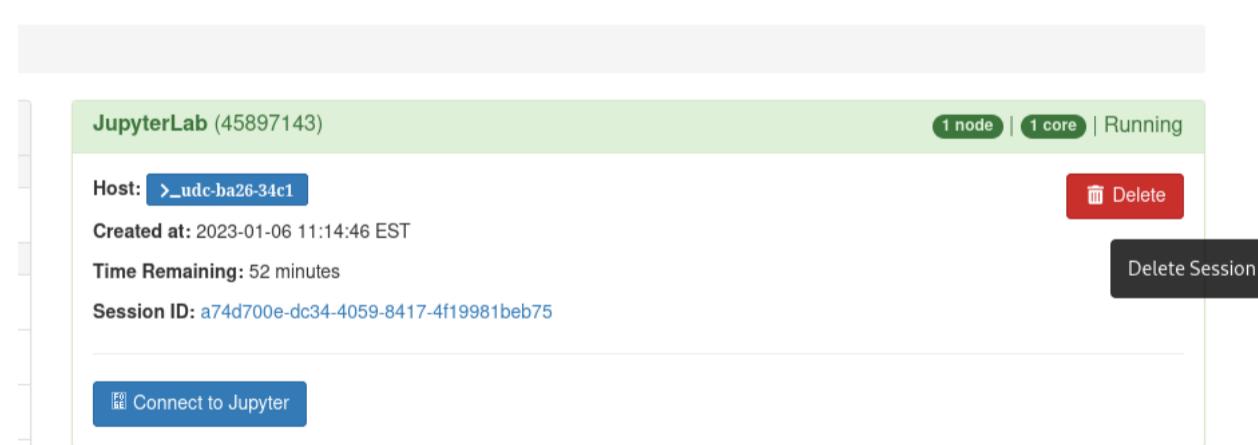
If you have not previously used the OOD JupyterLab interactive app, you must select a kernel before initiating the notebook. Once JupyterLab is set up, you can also start another notebook with a different kernel by selecting File->New Notebook. It will then show a dropdown with the kernels available to you.



Starting a new notebook.

If you are accidentally disconnected, you can go back to the OOD "My Interactive Sessions" tab and reconnect. However, anything left running in a cell may have been terminated. This is due to a limitation of Jupyter, not OOD or Rivanna, and does not apply to some of the other interactive apps.

Remember to delete your session if you finish early. Closing your browser tab does not end the session.



Ending a session.

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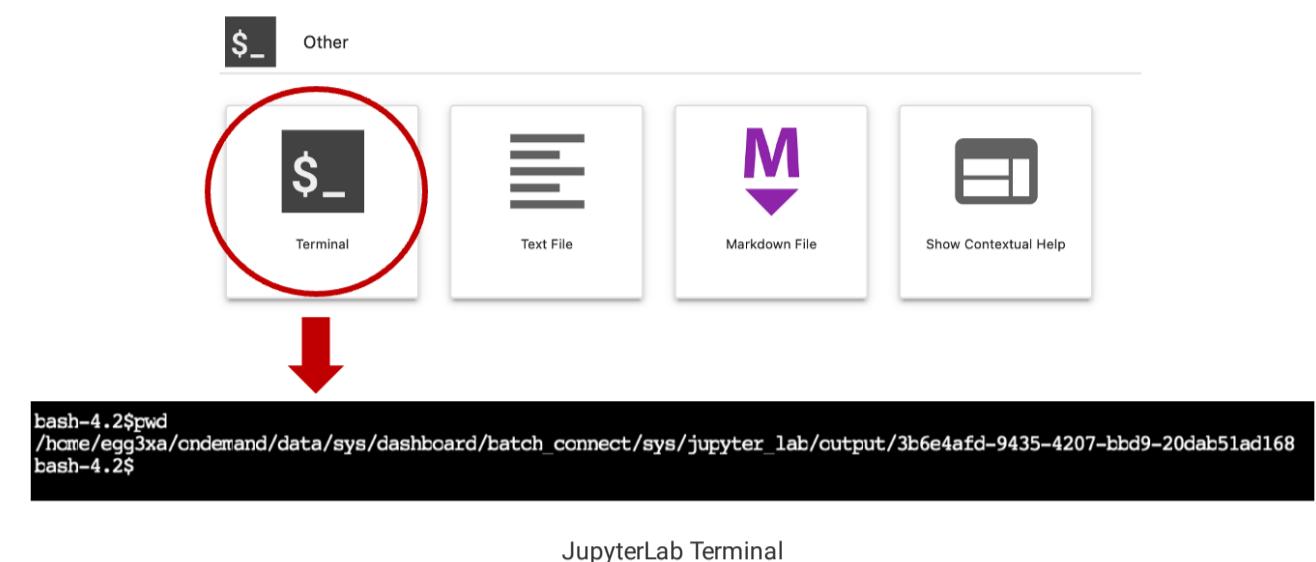
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JupyterLab Terminal

You are also able to access the terminal through a JupyterLab session.



Here, you can execute Linux commands to create custom conda environments and JupyterLab kernels. Additionally, you can access and run singularity containers through this functionality.

JupyterLab sessions will be saved in your

`/home/computingID/ondemand/data/sys/dashboard/batch_connect/sys/jupyter_lab/output/t/` directory on Rivanna; however, you can navigate to any part of the filesystem in the JupyterLab terminal.

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Rstudio Server

Rstudio Server is a standalone app like JupyterLab. Starting a session is very similar to JupyterLab, but the Webform differs slightly. Instead of kernel tiles, you will select a version of R from a dropdown menu from those available. In this example, the version is R 4.2.2.

RStudio Server

This app will launch RStudio Server an IDE for R on the Rivanna cluster.

NOTE: The plot package does not work properly in "RStudio 1.3.1073 - R 4.1.1". This is a known incompatibility with the R version + RStudio version. If your work requires the use of the plot package, please select "RStudio 2023.03.0 - R 4.1.2".

R version

RStudio 2023.03.0 - R 4.2.2

Rivanna Partition

Standard

- Dev - (1 core) For short sessions (1 hour) with no SU charge.
- Standard - (1-40 cores) Rivanna node in the standard partition.
- Instructional - (1-20 cores) Rivanna node in the instructional partition.
- GPU - (1-28 cores) Rivanna node that has NVIDIA GPU.
- Bii,Bii-gpu - (1-40 cores) Partition for Biocomplexity Institute and Initiative.
- Learn More - [Rivanna Queuing Policies](#)

Number of hours

1

Number of cores

1

Memory Request in GB (maximum 384G)

6

Allocation (Research or Class MyGroup) - lowercase-only

your_allocation

- MyGroup

Show Additional Options

No

Launch



Starting an Rstudio session.

Rstudio Server can continue running any active processes if your network is disconnected. Simply log back in to Open OnDemand, go to the My Interactive Sessions tab, and click **Launch** again. It will reconnect, not launch another session.

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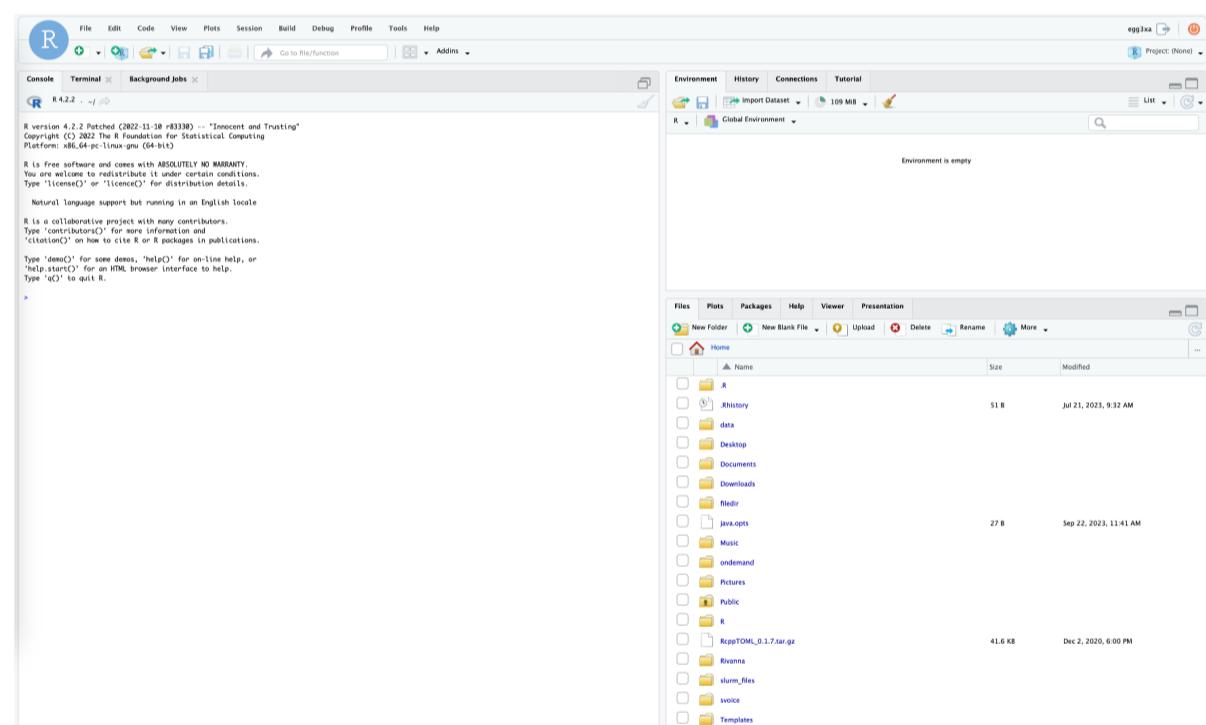
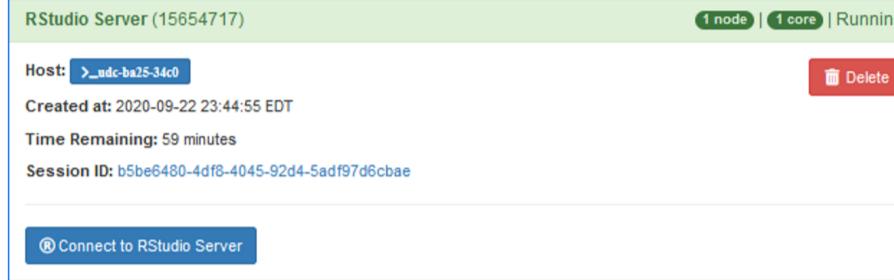
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Rstudio Session

Once you launch/submit your request, your job will wait in the queue until resources are available. You'll then be able to connect to your session:



Starting an Rstudio session.

Rstudio Server can continue running any active processes if your network is disconnected.

Simply log back in to Open OnDemand, go to the My Interactive Sessions tab, and click

Launch again. It will reconnect, not launch another session.

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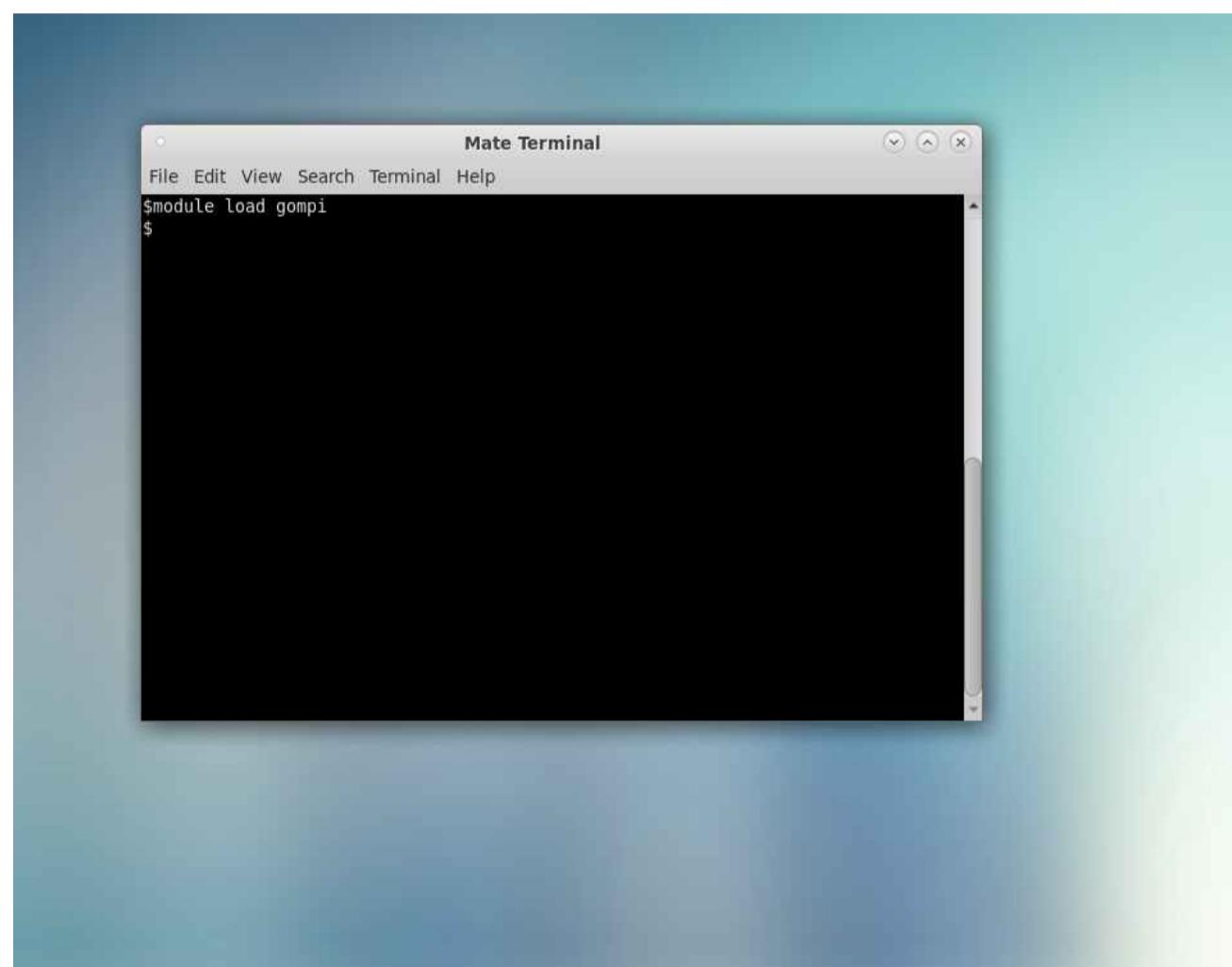
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Other Interactive Apps

Some other widely-used interactive apps are MATLAB and the Desktop.

Desktop

The most general OOD interactive app is the Desktop. It will start a desktop identical to the FastX desktop, but on a compute node rather than a frontend. From the desktop you can open a variety of applications from the menu, such as the Caja file manager. You can also open a terminal window and type any valid commands into it. In this illustration, the user has loaded a module to build a program for running. The OOD interactive desktop is the preferred method for interactive jobs.



The OOD Desktop.

MATLAB

The MATLAB interactive app starts a MATLAB Desktop environment on a Desktop (VNC). Similar to Rstudio Server, in the Webform you can choose a version of MATLAB from a dropdown menu. Once there, you are in a less complete desktop environment. Your files may not be visible on the Desktop, but you can access them from the Places menu or from the Caja (filing cabinet) icon in the ribbon at the top of the screen. If you exit the MATLAB Desktop, it will also exit the session.

Reconnecting

Both MATLAB and the Desktop will persist if your network is disconnected. Log back in to Open OnDemand, find your session from the My Interactive Sessions tab, then click [Launch](#) again.

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Field	Description
Number of cores	Used in parallel processing. Your code must be modified to take advantage of using multiple cores.
Memory Request in GB	When dealing with Big Data, you will need to increase the amount of memory. A good rule of thumb is to request 2 to 3 times the size of data that you are reading in or generating.
Work Directory	Allows you to change the working directory of a Jupyter Notebook to your /scratch folder.
Optional: Slurm Option	Allows you to provide advanced features, like requesting specific nodes or providing a reservation
Optional Group	Only needed if you are in more than 16 Rivanna groups. You may need to force Rivanna to see your allocation.
Optional: GPU type for GPU partition & Optional: Number of GPUs	Only needed if you are running on a GPU node. The "default" for GPU type will put you on the first available GPU node. For now, the number of GPUs should be 1.

Some fields on the Web Forms are blank, while others are set to default values.

The most important request will usually be the Memory Request.

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Exercise 1

Start a JupyterLab interactive session. Select the Python 3 kernel. If you are familiar with Python, you may write any code you wish. If you do not know Python, click on a cell and type the following

```
import numpy as np  
import matplotlib.pyplot as plt
```

Hit [Shift][Enter] (hold both keys at once) to run the cell, or from the Run menu choose Run Selected Cell.

In the next cell type

```
x=np.linspace(-1.*np.pi,np.pi,100)  
y=np.sin(x)  
plt.plot(x,y)
```

Run this cell.

Close the tab, return to My Interactive Sessions in the OOD Dashboard, and delete the interactive job.

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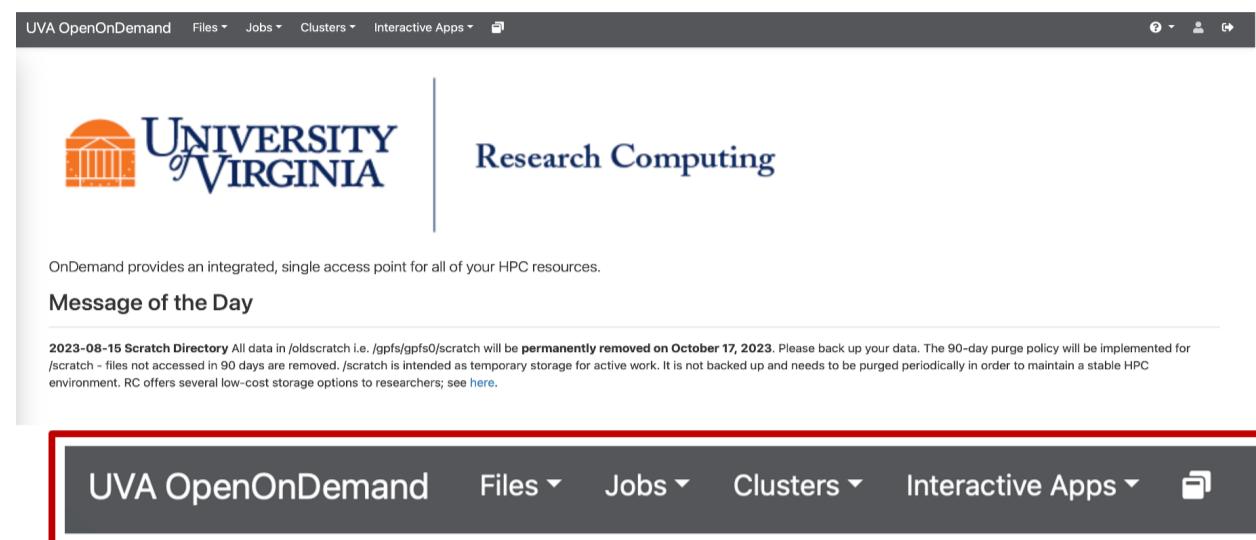
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Open OnDemand has many features accessible directly from the menu bar.



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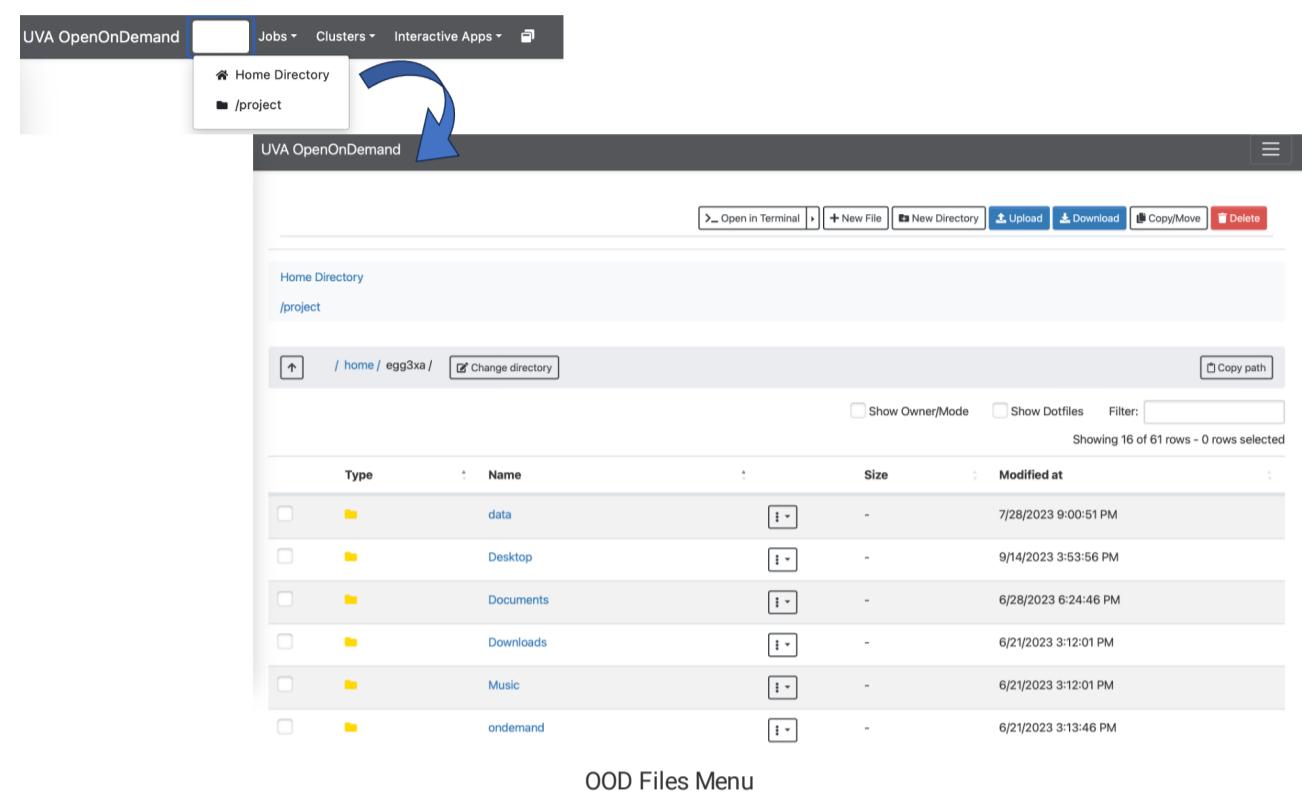
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Accessing Files on OOD

The “Files” tab on the menu bar gives access to all files in home or project (if applicable) directories.



Here, you can upload and download small files to and from Rivanna from your local computer. You can also create and delete new files and directories in addition to copying or renaming them. The Filter search bar searches for files or directories in the file system.

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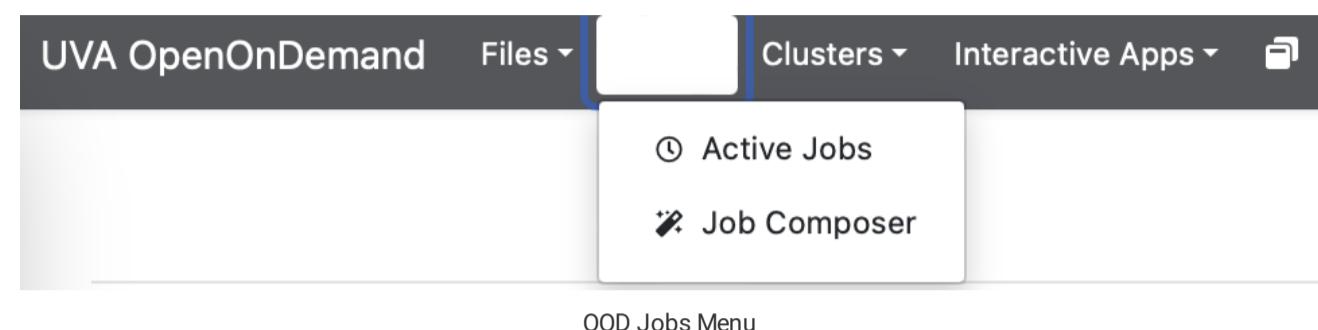
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Jobs on OOD

The “Jobs” tab on the menu bar allows you to submit and search for jobs on Rivanna.



OOD Jobs Menu

The “Active Jobs” tab shows all jobs currently running or queues on all partitions for all users. The Filter search bar allows you to narrow jobs by either user, queue, job name, job ID, or job status (running, queued, completed, etc).

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The job composer tab allows you to create and submit a job to run on Rivanna.

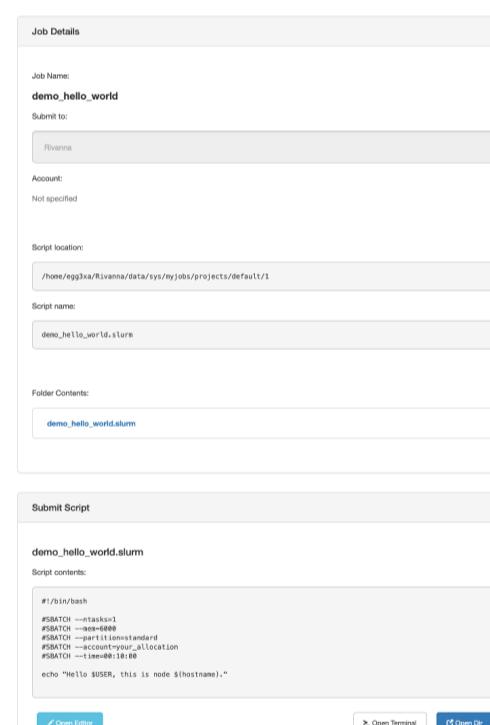


OOD Job Composer

Selecting the default template will automatically create a submission script called

`demo_hello_world.slurm` located in

`/home/computingID/Rivanna/data/sys/myjobs/projects/default/1` on the file system:



Default Template Job

Before submitting the job, `your_allocation` on the `#SBATCH --account=your_allocation` line must be replaced with the name of the allocation you're a member of. We will review editing files later. Once the correct allocation name is edited in, you can click "Submit" to queue your job on Rivanna. It will be given a corresponding Job ID, and once it's completed, the Folder contents will now contain a corresponding output file that contains the instructions from the submission script:

Folder Contents:

The screenshot shows a 'Folder Contents' section with two items: 'demo_hello_world.slurm' and 'slurm-53317409.out'. A large blue curved arrow points from the 'slurm-53317409.out' item down to a terminal window below. The terminal window displays the text 'Hello egg3xa, this is node udc-aw34-15c1.' followed by a line number '2'.

Default Template Output

There are several different job templates that can be run in addition to the default hello world option under New Job > From Template:

The screenshot shows a 'Template Options' page with a list of job templates. The columns are 'Name', 'Cluster', and 'Source'. The 'Name' column lists: demo_hello_world, demo-bowtie2, demo-copy-scratch, demo-matlab-job-array, demo-matlab-job-array-multicore, demo-matlab-mpi, demo-matlab-multicore, demo-matlab-serial, demo-python-job-array, and demo-python-mpi. All entries are under the 'Rivanna' cluster and 'System Templates' source. The page shows 10 entries per page, with a total of 25 entries. Navigation buttons at the bottom include 'Previous', '1', '2', '3', and 'Next'.

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The OOD Job Viewer

Open OnDemand allows you to check the status of your jobs easily. Open the Jobs tab and go to Active Jobs. The default view is All Jobs.

The screenshot shows the 'Active Jobs' table with the following columns: ID, Name, User, Account, Time Used, Queue, Status, and Cluster. There are 50 entries shown. Most jobs are in the 'Running' state, with some in 'Completed' or 'Pending' states. The 'Cluster' column shows Rivanna for all entries.

ID	Name	User	Account	Time Used	Queue	Status	Cluster
45596947	update_biotabanalyticst_covid19-wastewater-data.batch	bdk2pp	nsaac_covd19	00:00:00	bl	Completed	Rivanna
45550185	ood_jupyter	bl4zc	gordan	49:33:57	bl	Running	Rivanna
4561167	ood_rstudio	jz2rc	bl_stdad	05:39:05	bl	Running	Rivanna
45614891	ood_jupyter	kj5tl	bl_stdad	01:51:17	bl	Running	Rivanna
45614509	ood_jupyter	yhu2lk	bl_stdad	03:31:39	bl	Running	Rivanna
4555758	ood_jupyter	h2zdwk	bicomplexity	47:05:00	bl	Running	Rivanna
45509263	ood_jupyter	sawlnx	bicomplexity	122:51:59	bl	Running	Rivanna
4554717	ood_jupyter	asw3xp	bl_nsaa	52:06:27	bl	Running	Rivanna
45614824	ood_jupyter	zmfdru	bicomplexity	02:22:21	bl	Running	Rivanna
45609234	ood_rstudio	cpr9sw	bicomplexity	06:49:26	bl	Running	Rivanna
45545142	ood_jupyter	sv8nv	nsaac_covd19	52:49:19	bl	Running	Rivanna
45544368	ood_jupyter	pp2db	nsaac_covd19	53:49:29	bl	Running	Rivanna
45615313	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:24:18	bl-gpu	Completed	Rivanna
45615306	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:21:35	bl-gpu	Completed	Rivanna
45615292	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:21:36	bl-gpu	Completed	Rivanna
45615299	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:23:54	bl-gpu	Completed	Rivanna
45615340	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:12:34	bl-gpu	Completed	Rivanna
45615353	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:07:36	bl-gpu	Completed	Rivanna
45615346	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:08:19	bl-gpu	Completed	Rivanna
45615359	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:04:11	bl-gpu	Completed	Rivanna
45615331	ood_jupyter	y4dl	ds70034622	00:00:00	bl-gpu	Completed	Rivanna
45615290	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:26:09	bl-gpu	Running	Rivanna
45615341	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:14:20	bl-gpu	Running	Rivanna
45615334	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:16:59	bl-gpu	Running	Rivanna
45615327	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:20:02	bl-gpu	Running	Rivanna
45615320	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:22:04	bl-gpu	Running	Rivanna
45615318	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:23:11	bl-gpu	Running	Rivanna
45615355	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:09:28	bl-gpu	Running	Rivanna
45615354	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:09:48	bl-gpu	Running	Rivanna
45615347	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:11:56	bl-gpu	Running	Rivanna
45615348	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:11:56	bl-gpu	Running	Rivanna

Job status viewer in OOD.

You can filter to select subsets of the jobs, for example you can view only jobs in the **gpu** partition.

The screenshot shows the 'Active Jobs' table with the same structure as the previous one, but with a 'Filter' input set to 'gpu'. This results in fewer entries, mostly from the 'bl-gpu' queue, indicating successful filtering.

ID	Name	User	Account	Time Used	Queue	Status	Cluster
45615313	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:24:18	bl-gpu	Completed	Rivanna
45615306	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:21:35	bl-gpu	Completed	Rivanna
45615292	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:21:36	bl-gpu	Completed	Rivanna
45615299	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:23:54	bl-gpu	Completed	Rivanna
45615340	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:12:34	bl-gpu	Completed	Rivanna
45615353	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:07:36	bl-gpu	Completed	Rivanna
45615346	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:08:19	bl-gpu	Completed	Rivanna
45615359	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:04:11	bl-gpu	Completed	Rivanna
45615331	ood_jupyter	y4dl	ds70034622	00:00:00	bl-gpu	Completed	Rivanna
45615290	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:26:09	bl-gpu	Running	Rivanna
45615341	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:14:20	bl-gpu	Running	Rivanna
45615334	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:16:59	bl-gpu	Running	Rivanna
45615327	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:20:02	bl-gpu	Running	Rivanna
45615320	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:22:04	bl-gpu	Running	Rivanna
45615318	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:23:11	bl-gpu	Running	Rivanna
45615355	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:09:28	bl-gpu	Running	Rivanna
45615354	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:09:48	bl-gpu	Running	Rivanna
45615347	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:11:56	bl-gpu	Running	Rivanna
45615348	run_proc_gpu_VM.batch	hht9zt	bicomplexity	00:11:56	bl-gpu	Running	Rivanna

Viewing only the GPU partition.

You can also look at the status of only your own jobs by switching from All Jobs to My Jobs.

The screenshot shows the 'Active Jobs' table with a 'Filter' input set to 'Your Jobs'. It displays only two entries, both belonging to the user 'kah3f' in the 'standard' queue.

ID	Name	User	Account	Time Used	Queue	Status	Cluster
45897170	ood_desktop	kah3f	hpc_build	00:02:07	standard	Running	Rivanna
45897143	ood_jupyter	kah3f	hpc_build	00:15:22	standard	Running	Rivanna

Viewing only my jobs.

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Getting Job Details

In the OOD Job Viewer, clicking on the right arrow for a particular job will show details of the job if it is queued or running. Completed jobs will have no information available. Be patient as it can take a few moments for the information to be loaded. In this illustration the selected job is PENDING. The reason given is Resources, which means that no resources are available yet for this job.

guppy_bc 45614508	
Cluster	Rivanna
Job Id	45614508
Job Name	guppy_bc
User	nas8hj
Account	ont_sarscov2
Partition	gpu
State	PENDING
Reason	Resources
Total Nodes	1
Total CPUs	16
Time Limit	1:00:00:00
Time Used	0:00
Memory	49152M

Viewing only my jobs.

Completed jobs will be visible only for a short while as they are wrapping up and exiting.

If an error occurs, try reloading the page.

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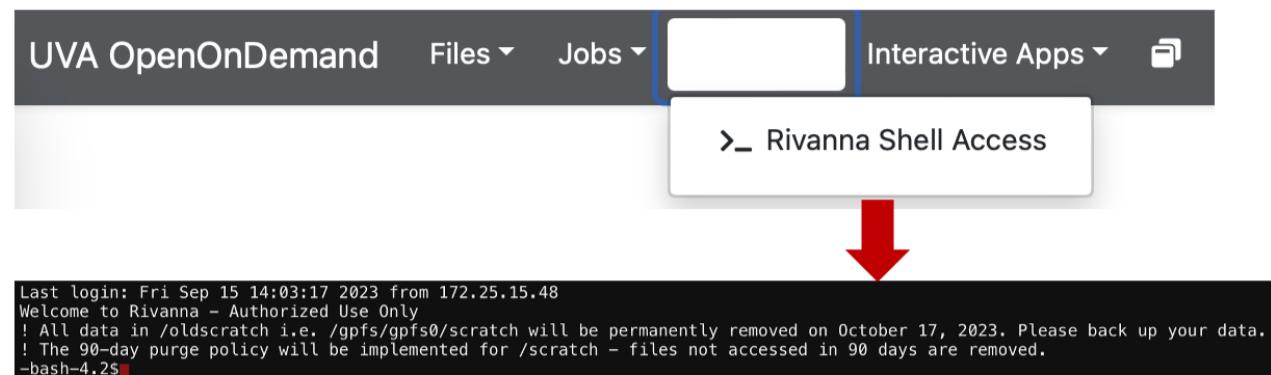
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Rivanna Shell Access

The “Clusters” tab on the menu bar open a new browser tab with a Linux command line interface for shell access:



Command line Shell Access

Here, you are able to upload and download small files to and from Rivanna from your local computer. You can also create and delete new files and directories in addition to copying or renaming them. The Filter search bar searches for files or directories in the file system.

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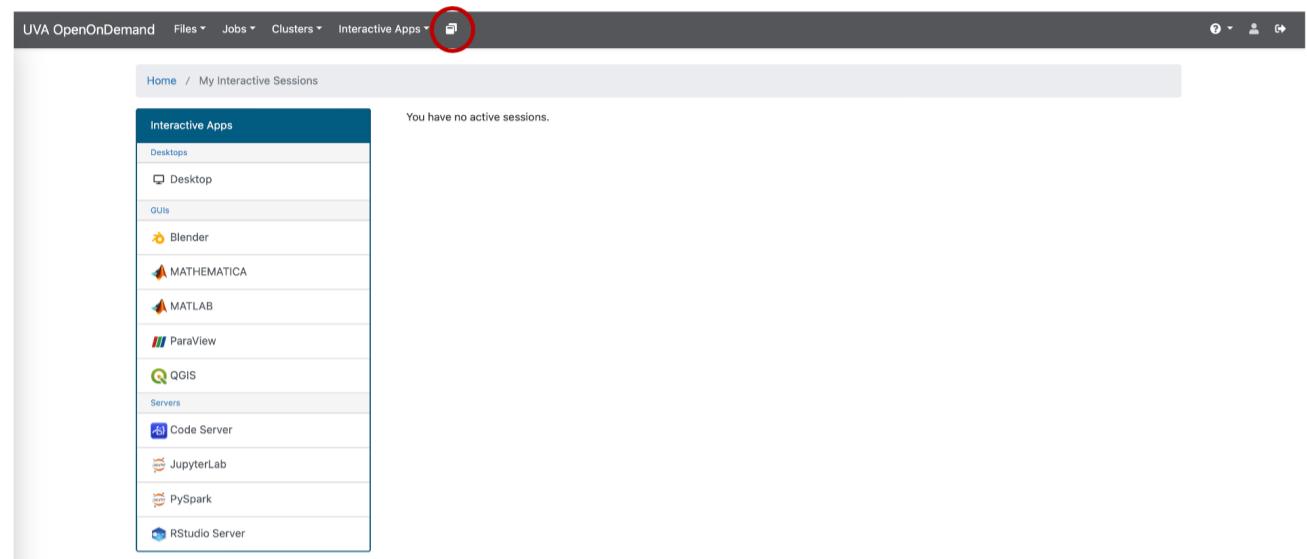
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This tab will show you running, pending or completed interactive sessions from the OOD interface.



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Useful Commands

Sometimes it's useful to check how many SUs are still available on your allocation. The `allocations` command displays information on your allocations and how many SUs are associated with them:

\$ allocations			
Account	Balance	Reserved	Available
robot_build	25000	0	25000
gizmonic-testing	921.952	0	921.952
crow-lab	928826	6236	922590
gypsy	0	0	0

Allocations

running `allocations -a <allocation_name>` provides even more detail on when the allocation was last renewed and its members.

One way to check your storage utilization is with the `hdquota` command. This command will show you how much of your home, scratch, and project (if applicable) storage are being utilized. Below is the sample output for `hdquota`:

Type	Location	Name	Size	Used	Avail	Use%
home	/home	egg3xa	50G	7.1G	43G	15%
Scratch	/scratch	egg3xa	12T	295M	12T	1%

Disk Usage

This is a useful command to check whether or not you're running out of storage space or to see where files need to be cleaned up. For more detailed information on disk utilization you may also use the `du` command to investigate specific directories.

To gain information on the different queues you can type `qlist` on the command line:

Queue (partition)	Total Cores	Free Cores	Jobs Running	Jobs Pending	Time	SU Charge
bii	4640	4316	55	109	7-00:00:00	1
standard	4080	1810	277	8	7-00:00:00	1
dev	160	119			1:00:00	0
parallel	4880	3056	10	15	3-00:00:00	1
instructional	480	319		1	3-00:00:00	1
largemem	144	120	3	2	4-00:00:00	1
gpu	1876	1194	89	28	3-00:00:00	3
bii-gpu	608	564	4	1	3-00:00:00	1
bii-largemem	288	264			7-00:00:00	1

Queues

This will show the list of partitions, their occupancy, and the SU charge rate. You can type `qlimits` for information on each queue's limits:

Queue (partition)	Maximum Submit	Maximum Cores(GPU)/User	Minimum Cores/Job	Maximum Mem/Node(MB)	Maximum Mem/Core(MB)	Default Mem/Core(MB)	Maximum Nodes/Job	Minimum Nodes/Job
bii	10000	cpu=400		354000+		9400	112	
standard	10000	cpu=1000		384000+	9600	9000	1	
dev	10000	cpu=16		384000	9000	6000	2	
parallel	2000	cpu=1500	4	384000	9600	9000	50	2
instructional	2000	cpu=20		384000	9600	9000	5	
largemem	2000	cpu=32		1500000	64000	60000	2	
gpu	10000	gres/gpu=32		128000+	32000	6000	4	
bii-gpu	10000			384000+		9400	12	
bii-largemem	10000			1500000		31000	2	

Finally, the `sinfo` command will provide some more detailed information on the health of each queue and the number of active nodes available. These commands can be useful in diagnosing why a job may not be running, or in better understanding queue usage for more efficient job throughput. More information on hardware specifications and queue information can be found on our [website](#).

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Exercise 2

Start an Open OnDemand File Explorer tab. In your home directory, create a new file. Use the Editor to enter the following text:

I came in with Halley's Comet in 1835. It is coming again next year, and I expect to go out with it. It will be the greatest disappointment of my life if I don't go out with Halley's Comet. The Almighty has said, no doubt: "Now here are these two unaccountable freaks; they came in together, they must go out together."

-Mark Twain

Name the file whatever you wish. Make a new folder "Quotes." Move the file to this directory.

Go to the FastX desktop and open Caja (the filing-cabinet icon, or from the System Tools menu). Navigate to your new directory. Change the name of the file. Use whatever method you prefer (right-click or F2 key). Still in Caja, copy the file. Give the copy the original name you choose. Move it to your Desktop.

Return to your Desktop in OOD and delete the file there.

On FastX, return to the Quotes directory. Open the file with Pluma, and after "Mark Twain" add ", 1909".

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Working with Files

Files are the foundation of working with Rivanna. We need to be able to

- Transfer files to and from Rivanna
- Edit text files
- Create files through the software we run

Each user has a **home** location and a **scratch** location. When you log in you will be in the **home** location. For now we will assume you will work with files in your home folder. We will discuss the scratch folder later.

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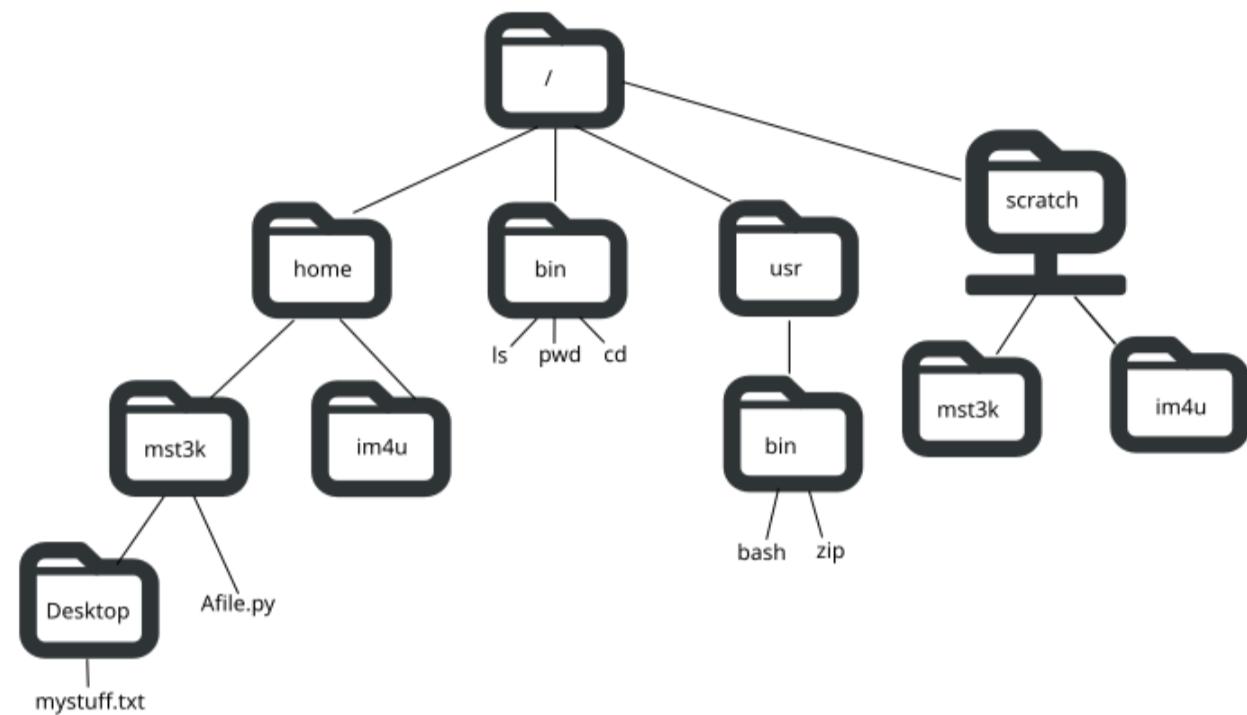
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Paths in Linux

Rivanna runs the Linux operating system. File paths start from *root*, denoted with a forward slash (/). The layout of the folders/directories is like an upside-down tree.



Schematic of folders on Rivanna. Only some files and folders shown.

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File Paths

Every file has a full name called its *path*. The path provides the operating system with the exact location of the file, relative to some starting point.

Examples:

- Windows C:\Users\mst3k\Desktop\mystuff.txt
- Mac OS /Users/mst3k/Desktop/mystuff.txt
- Linux (usually) /home/mst3k/Desktop/mystuff.txt

These paths traverse through some *folders*, which in Linux are often called **directories**, to arrive at the file mystuff.txt

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Transferring Files

You have several options for transferring data onto your home or scratch directories.

- Use a drag-and-drop option with [MobaXterm](#) (Windows) or [Filezilla](#) (Mac OS and Linux).
- For small files, use the Upload and Download buttons in the Open OnDemand FileExplorer App.
- Use the scp command.
- Use the web browser in the FastX desktop to download data from UVA Box or other cloud locations.
- Use the git clone command to copy git repositories
- Set up a [Globus](#) endpoint on your laptop and use the Globus web interface to transfer files. See <https://www.rc.virginia.edu/userinfo/globus/> for details.

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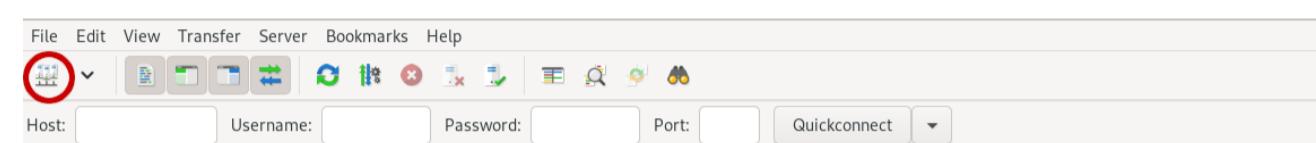
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Transferring with Graphical Clients: Mac OS and Linux

Filezilla

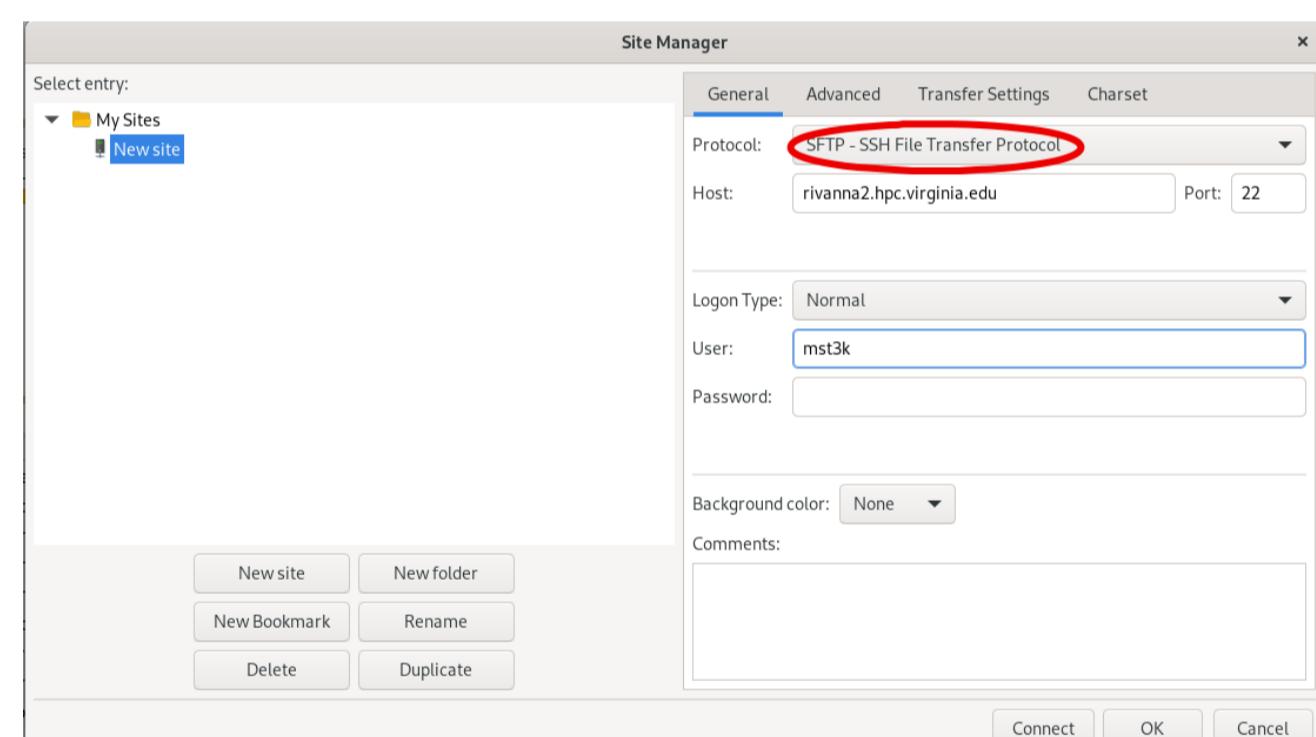
This illustration is from a Linux computer. Mac OS is similar.

First click the Site Manager icon in the upper left.



Site Manager

Select New Site. Rename it. Fill in the text boxes and dropdown. Be sure to select SFTP in the Protocol box. As for MobaXTerm, we recommend using a specific host name. Click **OK** to save and **Connect** to initiate the connection. A multiple-pane window similar to that of MobaXTerm will open.



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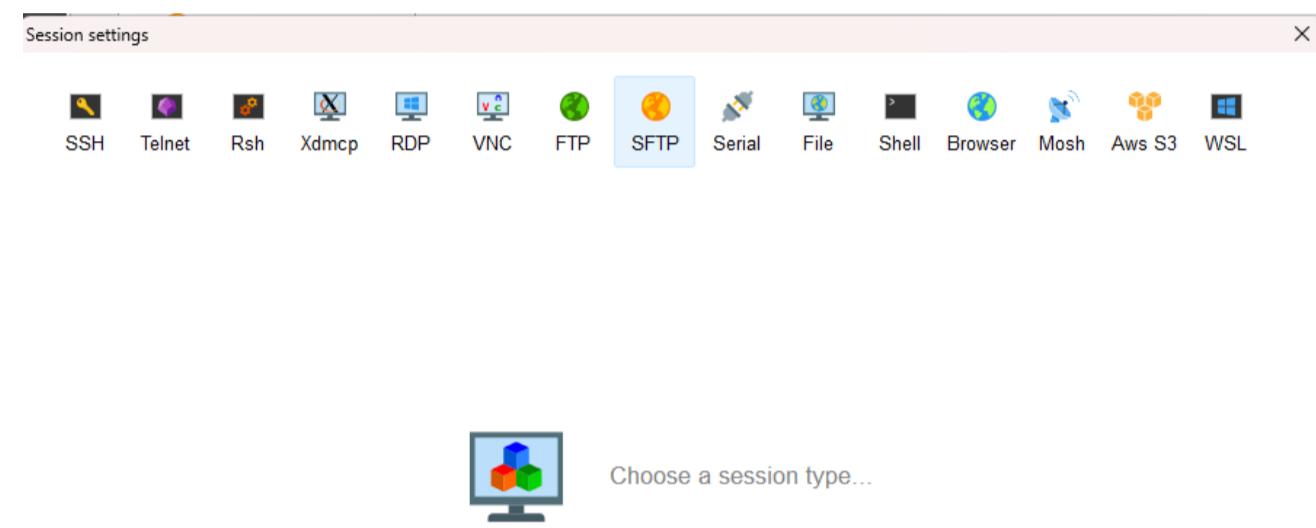
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Transferring with Graphical Clients: Windows

MobaXterm

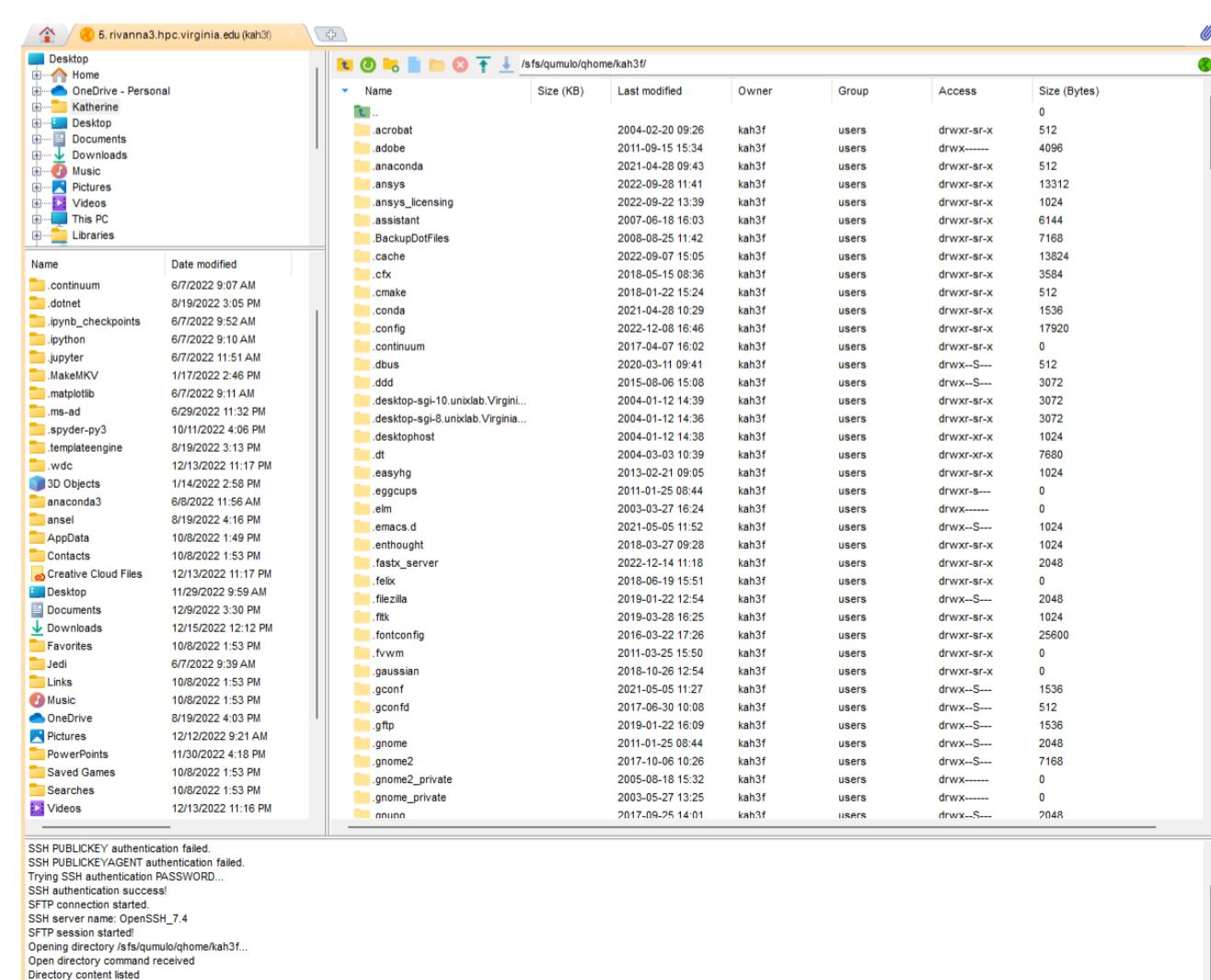
Start an SFTP session in MobaXterm. Use one of the specific hosts

[rivanna1.hpc.virginia.edu](#), [rivanna2.hpc.virginia.edu](#), [rivanna3.hpc.virginia.edu](#)



New SFTP session in MobaXTerm

A double-paned window will open. Drag and drop files between your local machine and the remote server.



Drag and drop

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Transferring with Globus

Globus

Globus is a non-profit service for secure, reliable research data management developed and operated by the University of Chicago and Argonne National Laboratory, supported by funding from the Department of Energy, NSF, and the NIH. With Globus, subscribers can move, share, & discover data via a single interface – whether your files live on a supercomputer, lab cluster, tape archive, public cloud or your laptop, you can manage this data from anywhere, using your existing identities, via just a web browser.



Advantages of Using Globus

Globus provides a secure, unified interface to your research data. Use Globus to “fire and forget” high-performance data transfers between systems within and across organizations.

Installing Globus

To transfer data to and from your computer, you will first need to install Globus Personal Connect. The following links provide instructions for installing Globus Personal Connect based on your machine’s operating system.

Platform	Installation instructions
Mac	https://docs.globus.org/how-to/globus-connect-personal-mac
Linux	https://docs.globus.org/how-to/globus-connect-personal-linux
Windows	https://docs.globus.org/how-to/globus-connect-personal-windows

Transferring Files

Files are transferred with the Globus File Manager Web App. There are three ways to get to the app:

1. Go straight to <https://app.globus.org/file-manager>
2. Go to <https://www.globus.org/> > Log In (top right corner)
3. Click Globus icon in Toolbar > Web: Transfer Files

Once the app is open you can choose collections to transfer data between.

Sharing Data with Collaborators

Globus users are able to share data with anyone with a Globus account. All UVA Rivanna and Ivy users have Globus accounts (authenticate with Netbadge).

External collaborators don’t need to be affiliated with an institution using Globus in order to share data with them. Anyone can create a Globus account using @globusid.org

More information on using Globus can be found on our learning [website](#) and from our [documentation](#).

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Creating and Deleting Files

There are three quick ways to work with files.

- The Open OnDemand File Explorer.
- If logged in through FastX, you can use the “Caja” file manager. It can be accessed through the filing-cabinet icon in the ribbon at the top, or via the Applications->System Tools menu. Caja works very similarly to Windows Explorer and the Mac Finder, but is somewhat more limited. It should be simple to use. The Open OnDemand file manager shows only one location at a time, whereas Caja, like Explorer or Finder, can open multiple windows. Note: you will not be allowed to do anything as “Administrator.”

i In Open OnDemand and Caja, rather than trying to navigate to your /scratch directory, use Go To (OOD) or Go->Location (Caja) and type the path `/scratch/mst3k`, using your own ID rather than `mst3k`.

Creating Files and Folders

- Open OnDemand: click the New File (file) or New Dir (folder) button and provide the name. You may also provide a path.
- In FastX with Caja: For a new file go to the File->Create Document menu. For a folder use File->Create Folder.
- In FastX you can use an editor such as `pluma`, which is accessible through the Applications->Accessories menu, using its File->New menu item. You can then use the editor to add content to the file.

Deleting Files and Folders

- In the Open OnDemand File Explorer, select the file or folder, then click the red Delete button. It will request confirmation.
- In the “Caja” file manager on FastX, right-click and Delete. Since the space in your home directory is limited, we recommend not moving to Trash.

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Copy, Rename, and Move Files

Renaming Files and Folders

- In the Open OnDemand File Explorer, click on Files on the Dashboard and click the file or folder you want to rename. Find the menu (three vertical dots) to the right of the file name. Click Rename.
- In the “Caja” file manager on FastX, select the file or folder. The combination of clicking on the icon and hitting the F2 key, should work on most keyboards as it does for Windows. You can also right-click and choose Rename.

Moving Files and Folders

- In the Open OnDemand File Explorer, use the Copy/Move button in the upper right. Select the file or folder you wish to move. A dialog will open. In your navigation pane, go to the target folder. Click Copy in the dialog on the left.
- In the “Caja” file manager on FastX, if moving within the same parent folder, just drag the file or folder to the new location. If moving between folders that do not share a parent, open another Caja window. Cut the file or folder and paste to its new location.

Copying Files and Folders

- In the Open OnDemand File Explorer, use the Copy/Move button, but click on Copy rather than Move.
- In the “Caja” file manager on FastX, open another Caja window and drag the icon of the file or folder between them. Alternatively right-click and use the copy and paste menu items.

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Editing Files

Once we have our files on Rivanna, we may need to edit them. It is a good idea to edit your files directly on Rivanna, rather than editing on your local computer and then transferring them back and forth.

You can create files by the same process as editing an existing one; just select [New](#) if there is a menu.

You can use:

- The built-in editor in Open OnDemand. Click on Files on the Dashboard, highlight the file that you want to edit. From the dropdown menu next to the file name, select Edit. A simple editor will open. To create a file, navigate to the desired location, click the New File button, then edit that file.
- If logged in through FastX, you can use the [pluma](#) editor, which is accessible through the Applications->Accessories menu. You can also start it from a terminal with either its name [pluma](#) or as [gedit](#) (those are the same program).
- The MATE desktop in FastX also provides the semi-graphical editors [Emacs](#) and [GVim](#) in the same menu.
- In FastX, you can also use a programmer's interface such as VSCode, Spyder, or Rstudio. For extensive editing or running programs through environments such as VSCode, use the Open OnDemand [interactive app](#).

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Exercise 3

Now that we have covered the basics of OOD interactive apps, OOD functionality, and how to work with files, we will now put everything together to create a unique job submission script and run it through the job composer on OOD. In this example we will write a simple 'Hello World!' python script and a submission script to be run with the OOD job composer.

You'll need to create two files in your Desktop ([/home/computingID/Desktop](#)): `hello.py` and `hello.slurm`. You can use any text editor of your choice: FastX editors (pluma, gedit, etc.) or the OOD file editor. In `hello.py` add the following lines:

```
# Write hello 10 times
for i in range(10):

    print ("\n {} Hello World!".format(i+1))

print("\n\n")
```

Next, we will need a submission script to submit this code to run on a compute node. Open `hello.slurm` and add the following:

```
#!/bin/bash
#SBATCH --cpus-per-task=1
#SBATCH --mem=6000
#SBATCH --time=00:05:00
#SBATCH --partition=standard
#SBATCH --account=your_allocation

module purge
module load anaconda
python hello.py
```

Be sure to replace `your_allocation` with the name of the allocation you have access to.

Once these two files are created, you can use the job composer on OOD to submit `hello.slurm` to a compute node to run the python code.

Once the job has completed, you should see a `slurm-jobID.out` file in your Desktop. View the file and make sure its contents are what you expect.

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Getting Help

If you have questions you can visit one of our [online office hours](#) Zoom sessions. Click on the “Join us via Zoom” button when a session is open. Current hours are

Tuesdays: 3 pm – 5 pm

Thursdays: 10 am – noon

For specific help you can [submit a ticket](#) (this may open Netbadge).

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