

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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The Rivanna cluster

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# Terminology

- 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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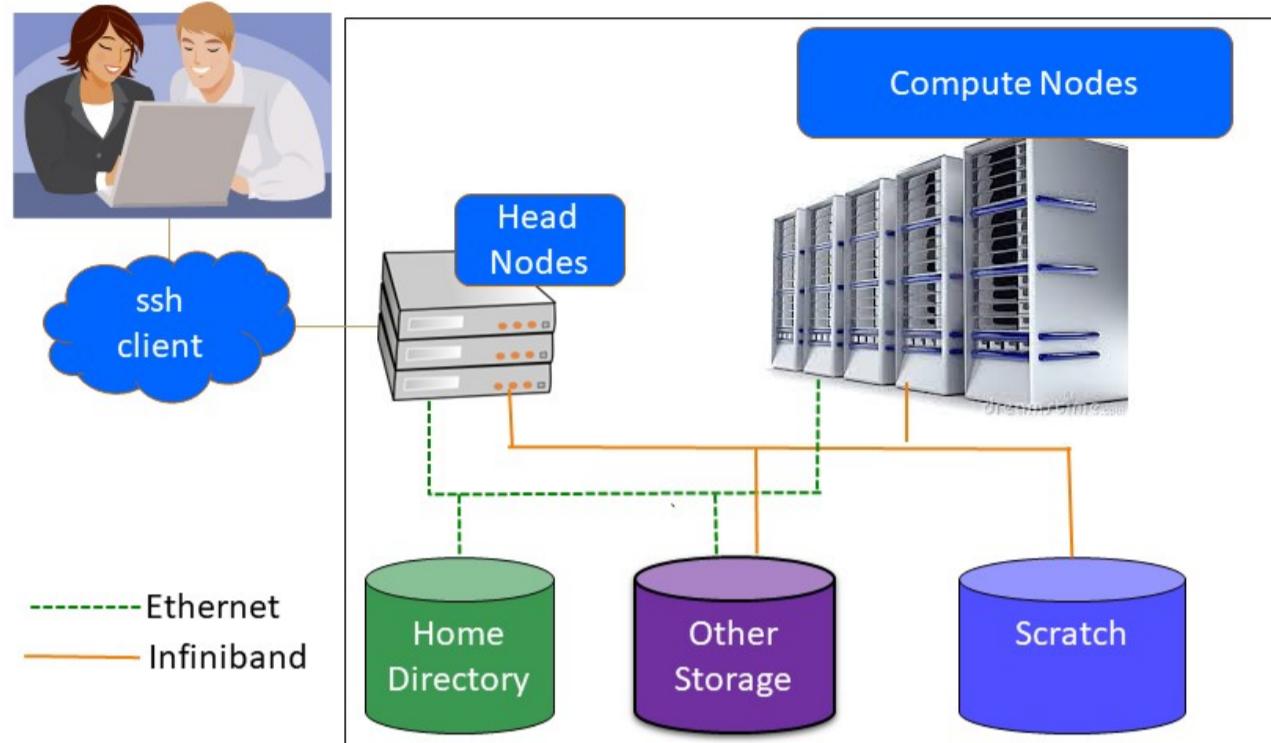
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A schematic illustration of a cluster

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# Allocations and Accounts

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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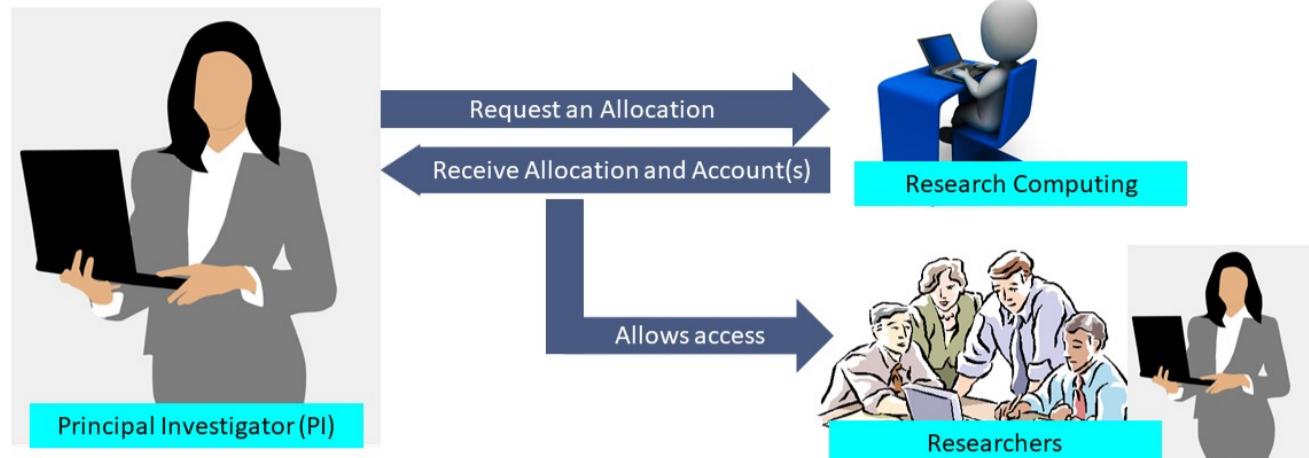
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# Login Accounts

- 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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# 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.

Powered by OnDemand

OnDemand version: v1.6.20 | Dashboard version: v1.35.3

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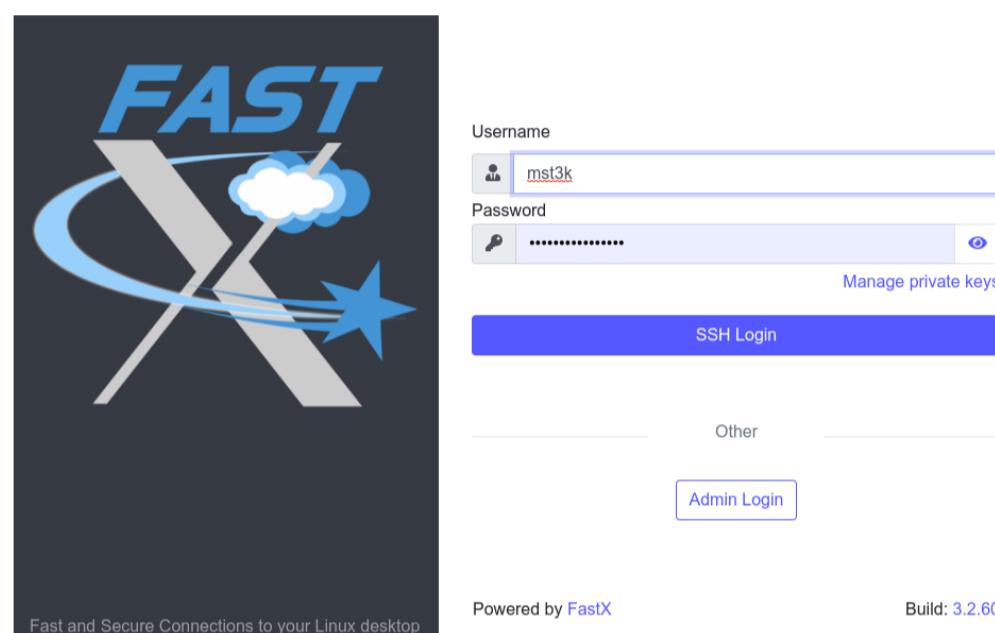
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# Connecting with FastX

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](http://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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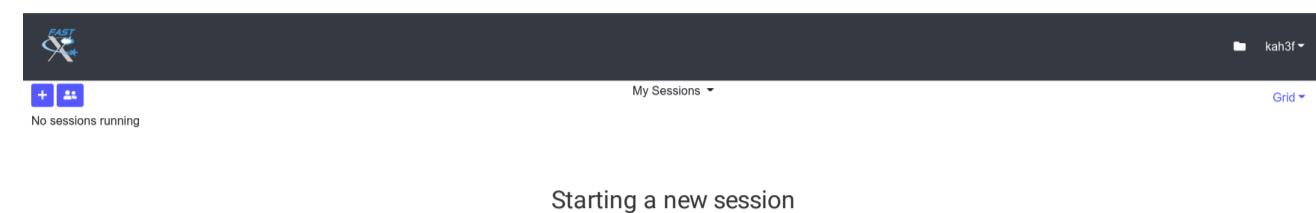
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FastX starts a session on a Rivanna frontend. A new session is started by clicking the  button.



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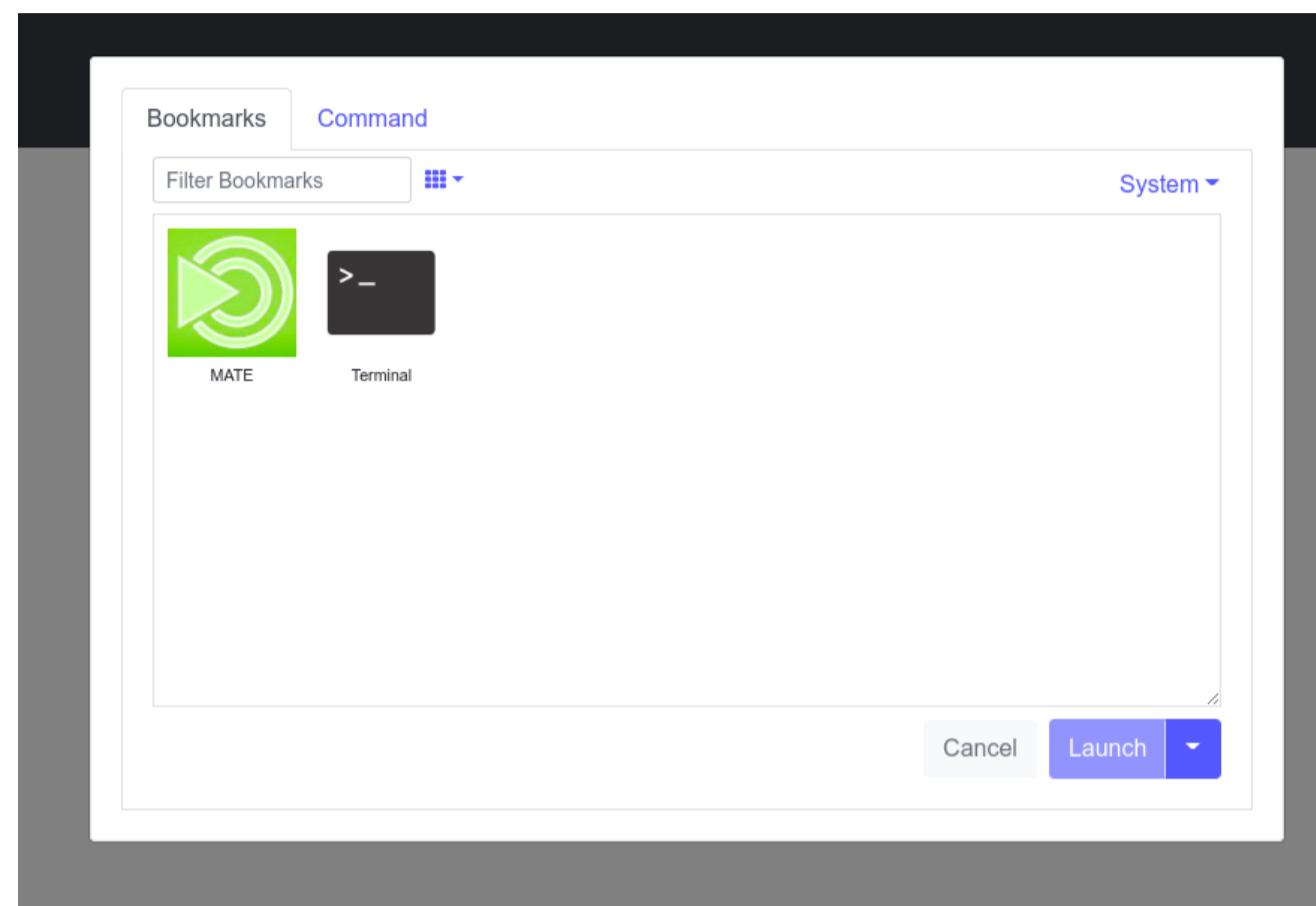
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Most users should chose the MATE session. Click the icon, then click the [Launch](#) button.



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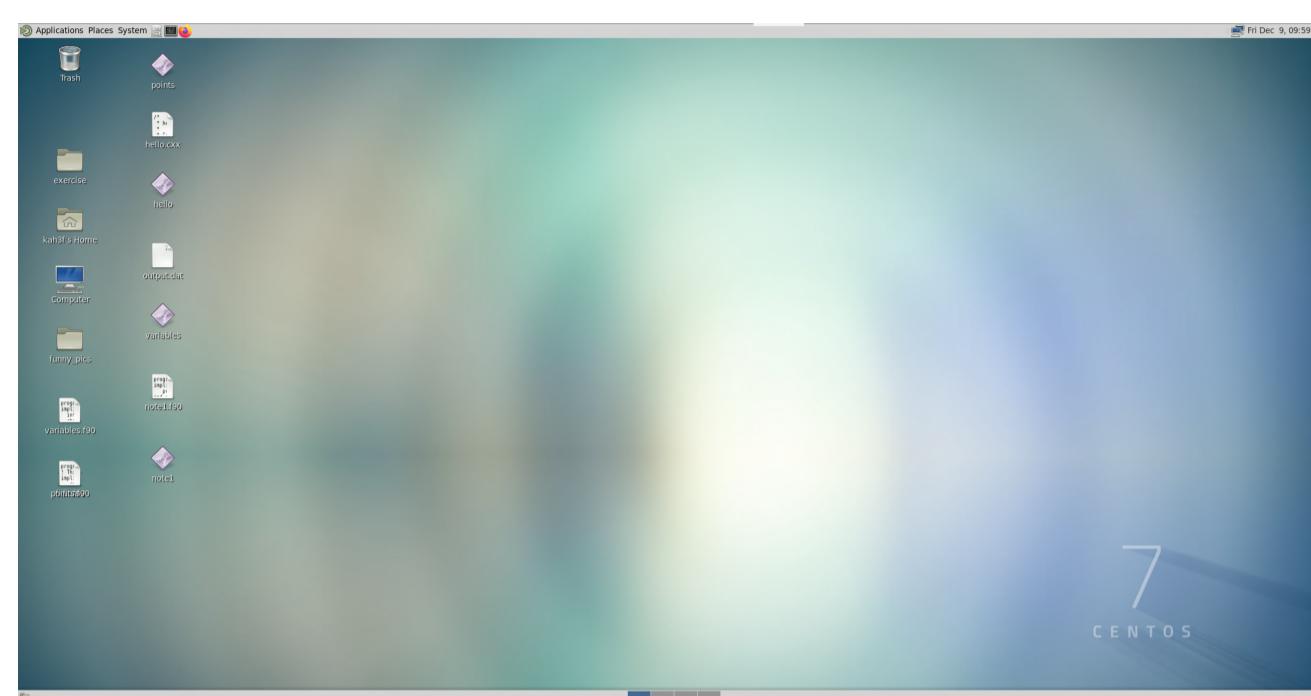
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A MATE desktop looks a little like an older Windows desktop. In the ribbon at the top are **Caja**, a file manager; a **Terminal** application, and the Firefox Web browser.



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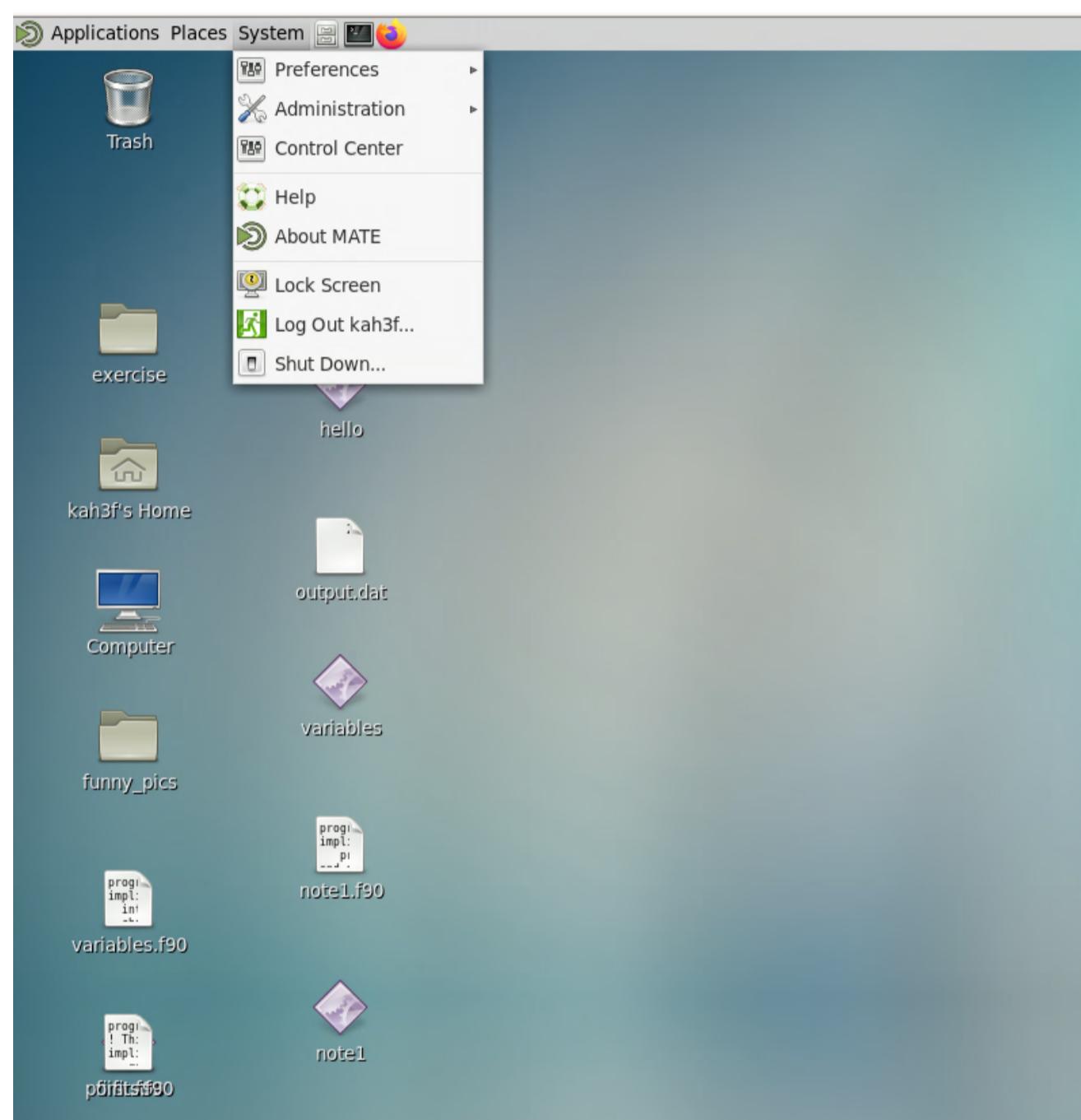
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# Logging Out of FastX

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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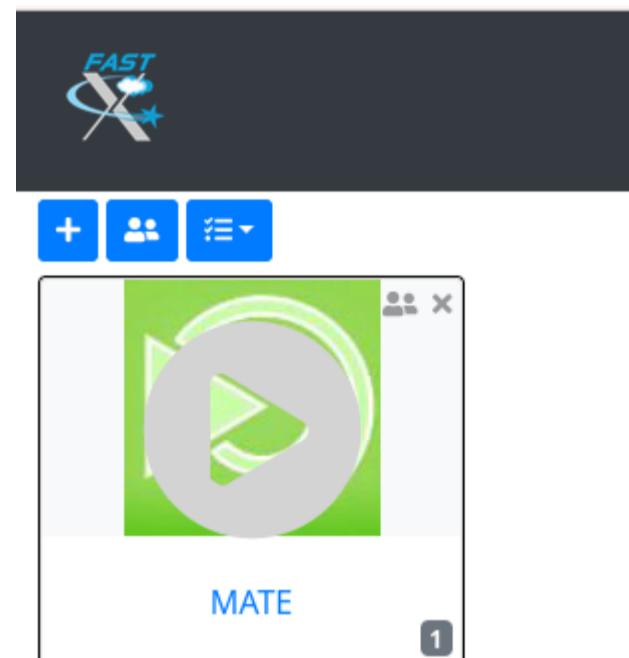
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# Terminating or Restarting FastX

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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# SSH

Finally, we can connect through the *command line* with `ssh`, the Secure SHell.

- Open OnDemand
  - From the Dashboard, select Cluster, then Rivanna Shell Access. This should log you in directly to a terminal.

## Linux and Mac OS

- Use a command line
  - `ssh mst3k@rivanna.hpc.virginia.edu`
- Substitute your own user id for `mst3k`
- We recommend installing [XQuartz](#) on Mac OS.

If XQuartz is installed, or you are using Linux, the command should be

```
ssh -Y mst3k@rivanna.hpc.virginia.edu
```

## Windows

- We recommend [MobaXterm](#)
- Choose an SSH session
  - Enter your user ID and optionally your password
  - Save the password if you wish
  - MobaXterm bundles the X windowing system so can start graphical apps.

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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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# 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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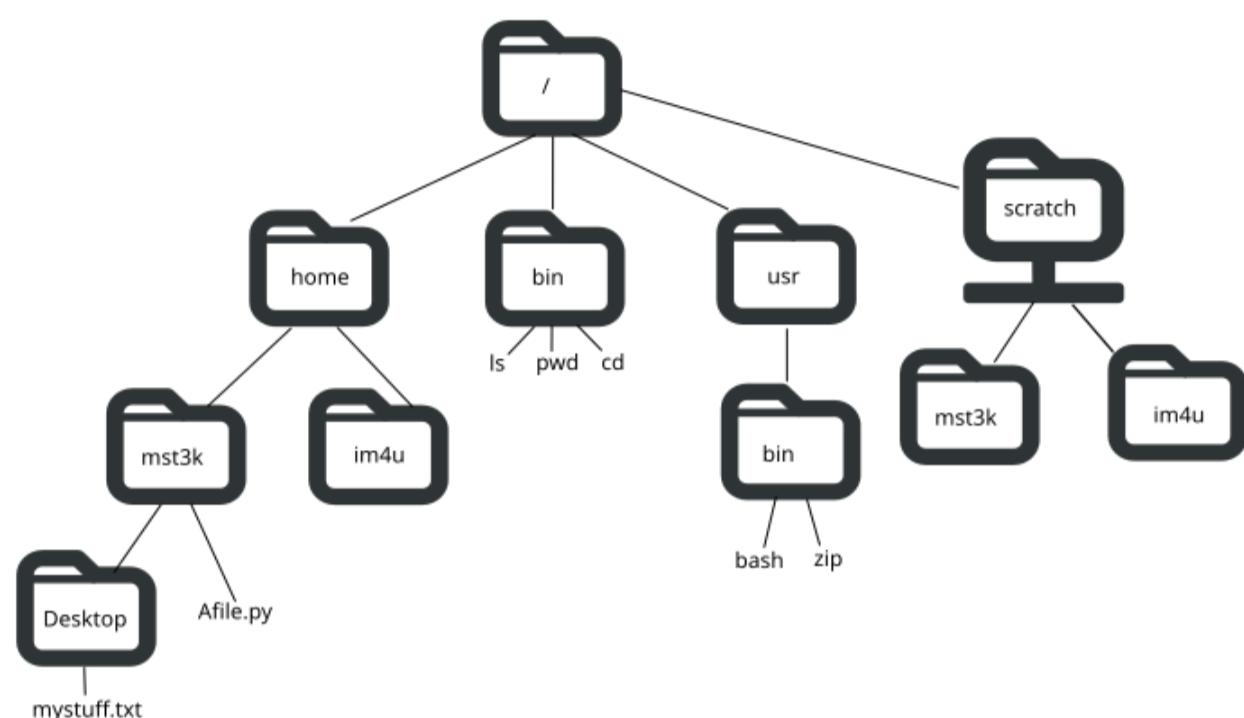
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# Paths in Linux

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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# 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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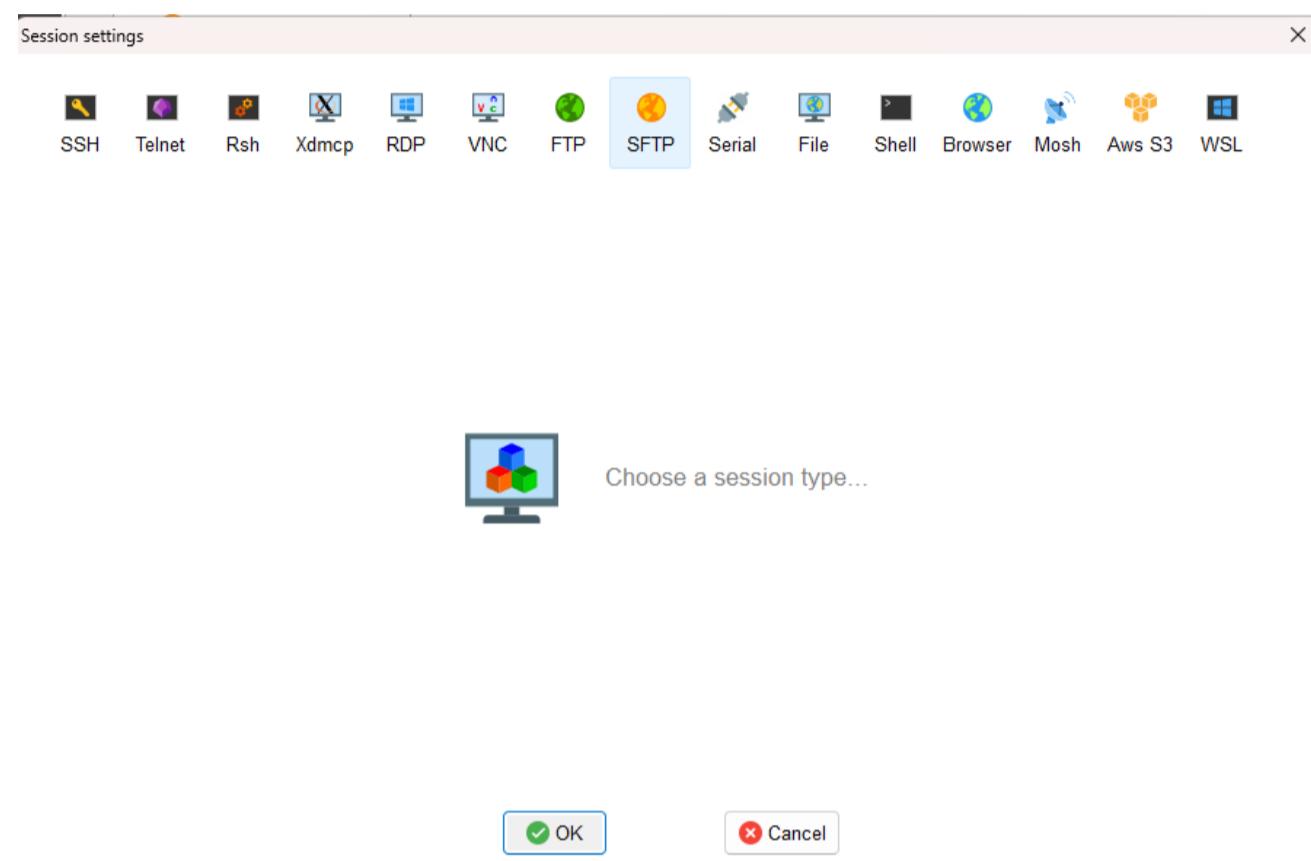
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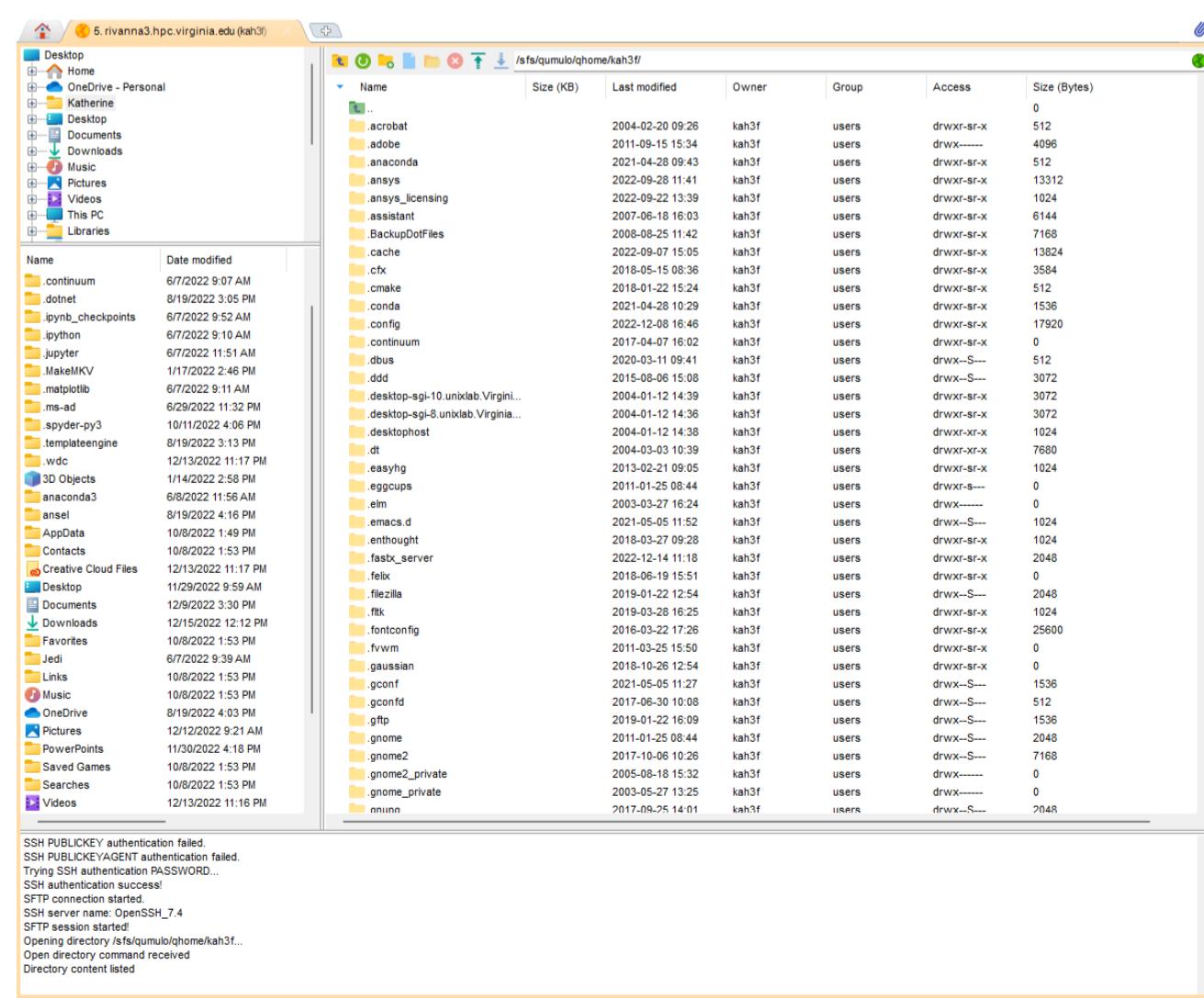
## MobaXterm

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

**rivanna1.hpc.virginia.edu, rivanna2.hpc.virginia.edu, rivanna3.hpc.virginia.edu**



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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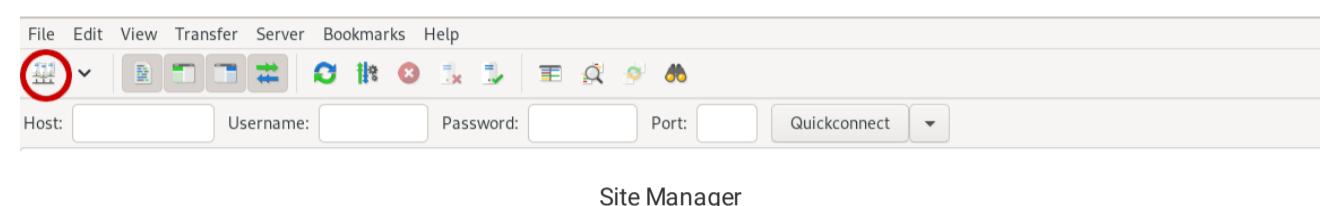
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## Filezilla

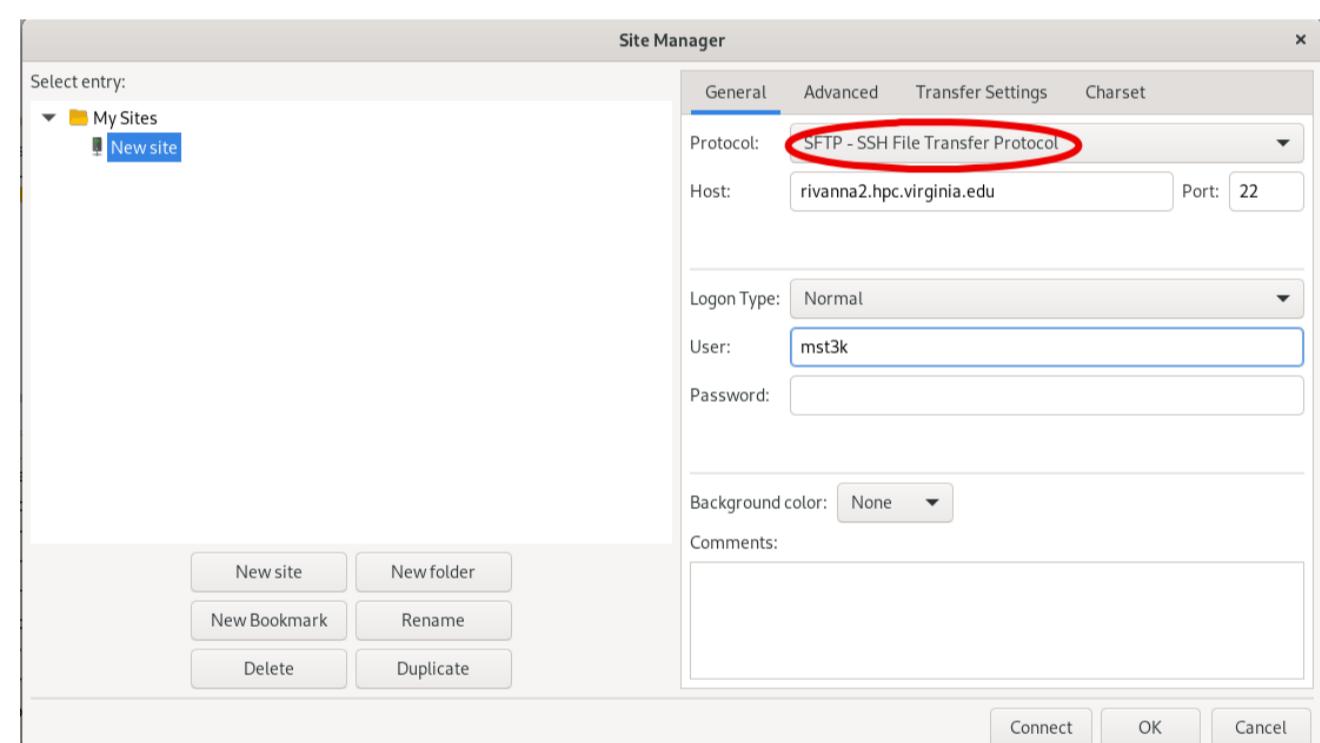
This illustration is from a Linux computer. Mac OS is similar.

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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# Transferring with Command-Line SCP

The syntax of the command-line `scp` is similar with all operating systems. Always execute it from your *local* machine to a rivanna frontend.

Transfer *from local to Rivanna*

```
scp path/to/file mst3k@rivanna2.hpc.virginia.edu:
```

Be sure to include the colon after the `edu`. The path will depend on the local operating system. This syntax copies the file into your home folder on Rivanna.

Transfer *from Rivanna to local*

```
scp mst3k@rivanna2.hpc.virginia.edu:path/to/file localpath
```

The path on Rivanna is relative to your home folder.

## Windows

Go to Settings->Apps->optional features and be sure [OpenSSH Client](#) is installed. This [site](#) has a good explanation of using command-line scp in both Powershell and cmd.exe. Of course you should substitute a Rivanna frontend for the Drexel computers.

## Mac OS and Linux

Open a Terminal window and type the `scp` command as shown above.

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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`.

- Use the command line.

## 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.
- If you are using a command line you can use a text editor like `vi` or you can use the `cat` command followed by the name of the new file. For a folder, type `mkdir dirname`.

## 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.
- From the command line, for a file type `rm filename`. For a directory type `rm -rf directoryname`.

**!** When deleting a file at the command line, it *will not* ask for confirmation unless you add the `-i` flag to the `rm` command.

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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.
- From the command line type `mv oldname newname`.

## 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.
- From the command line type `mv oldpath newpath` (that is, include the path and not just the file/folder name).

## 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.
- From the command line type `cp oldpath newpath` (that is, include the path and not just the file/folder name) if you wish to copy the file into a different folder. If copying to the same folder, `cp current_name copy_name` is sufficient.

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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](#).
- When in a Terminal, through ssh or FastX, use a text editor such as vi or nano.
  - vi uses keyboard commands and may take a while to learn.
  - nano is a very basic editor.

To launch vi or nano, type

```
vi myfile.txt
```

or

```
nano myfile.txt
```

**i** Nano is fairly self-explanatory but documentation is [here](#). On Rivanna **vi** is equated to **vim** which has documentation [here](#). GVim is an editor built on top of vim with some friendlier features, such as easier navigation. Vi can be used from a text-based terminal, including the Open OnDemand terminal app.

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# Exercise 1

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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# 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.

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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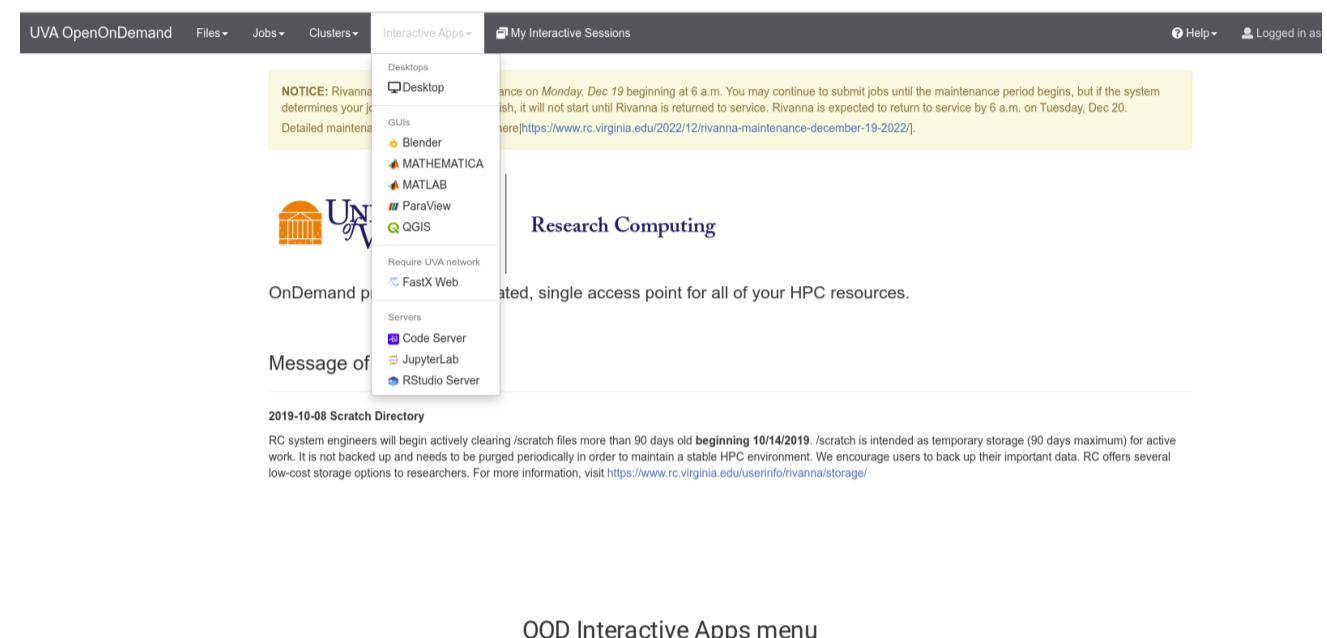
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# The OOD Interactive Apps Menu

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.

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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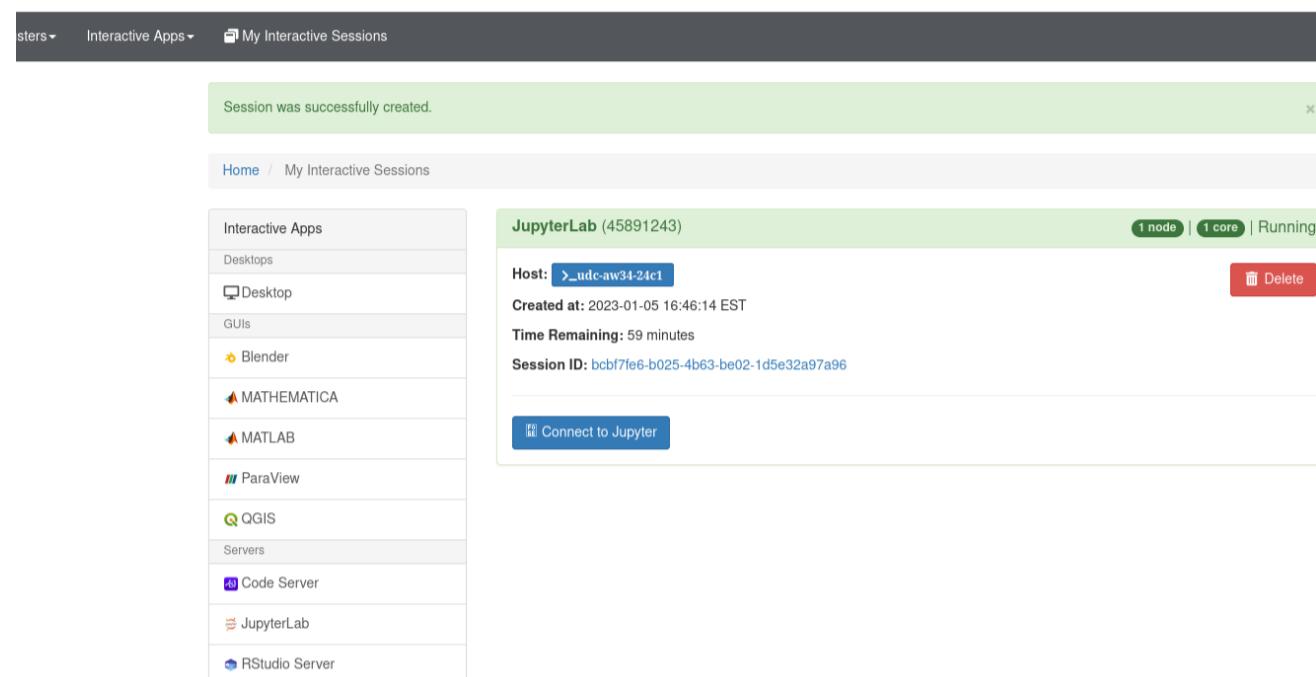
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# Launching an Interactive Session

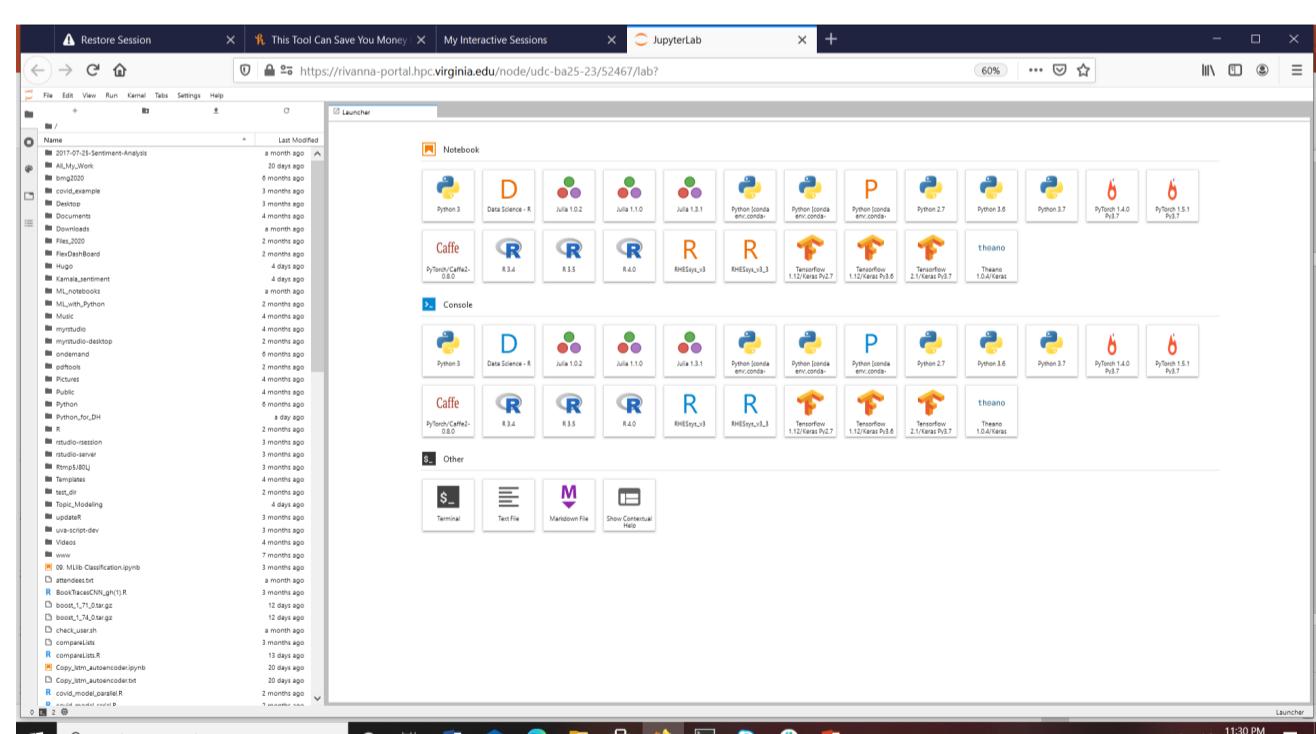
When you submit a request for an interactive app, it will be placed into the partition you specified, where it will wait until resources become available. Requests with higher resource requests (more cores, more memory, more time) may wait longer.

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.



Start screen for JupyterLab

If you have connected previously, it may start from your earlier status and you will not see the tiles.

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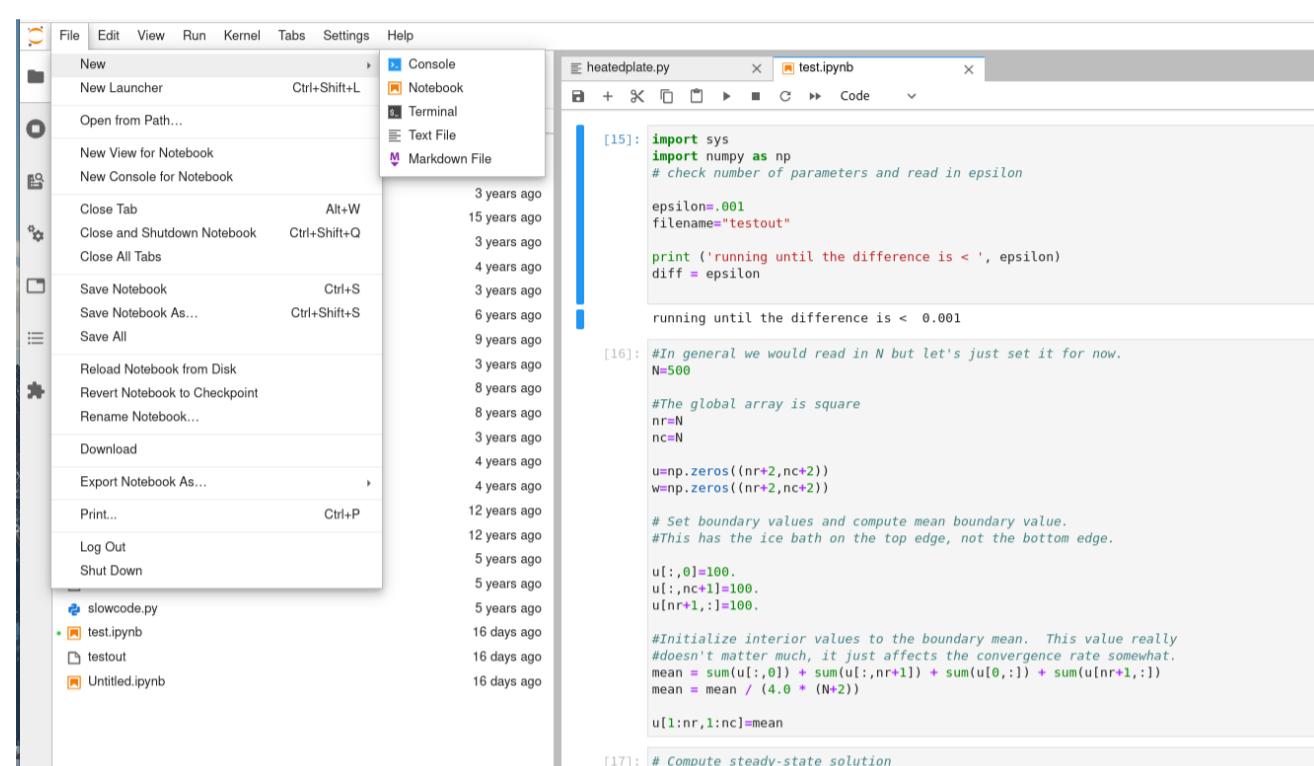
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# Using and Closing an Interactive Session

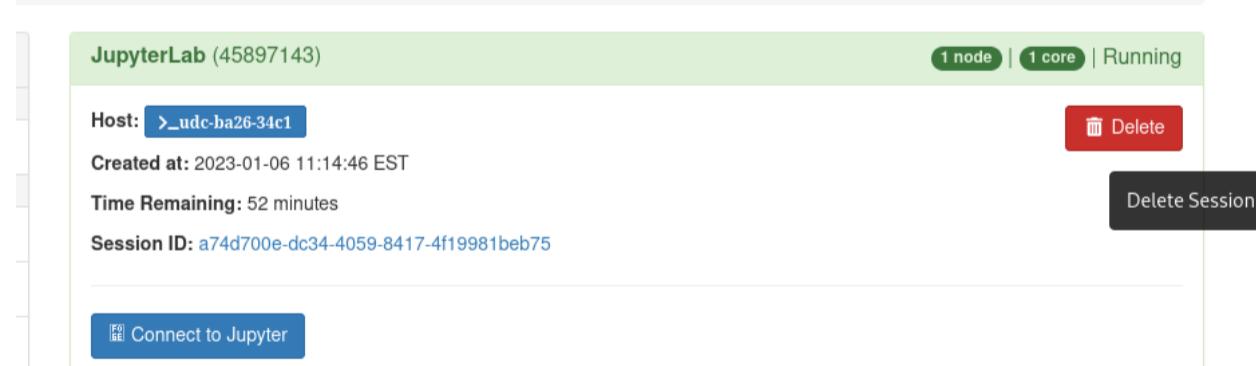
If you have not previously used the OOD JupyterLab interactive app, you must select a kernel before initiating the notebook. Once JupyterLab is set up, you can also start another notebook with a different kernel by selecting File->New Notebook. It will then show a dropdown with the kernels available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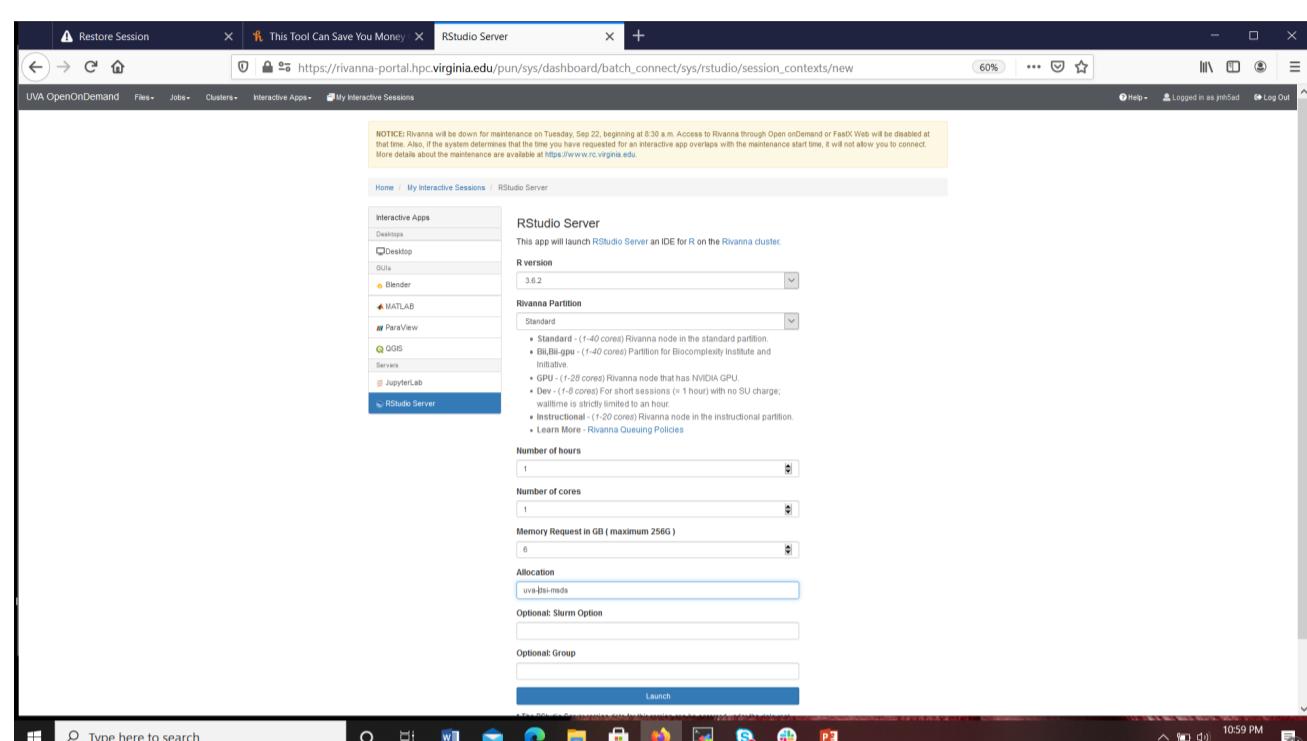
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# Rstudio Server

Rstudio Server is a standalone app similar to 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 3.6.2.



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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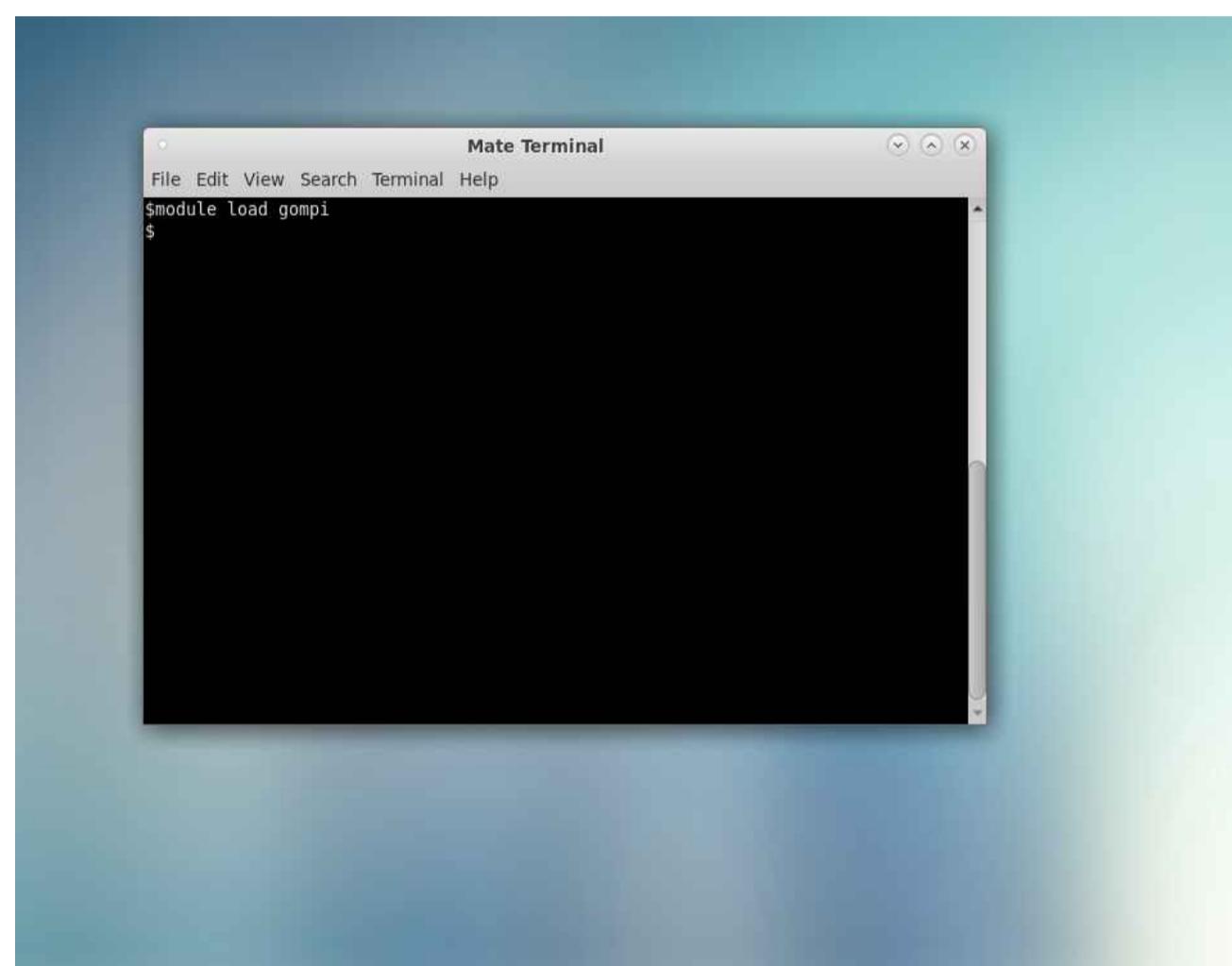
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# Other Interactive Apps

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 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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# 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.

Active Jobs											
Show	50	entries									
ID	Name	User	Account	Time Used	Queue	Status	Cluster				
> 45596947	update_biotrnanlytics_covid19-wastewater-data.batch	bdk2pp	nsaac_covid19	00:00:00	bl	Completed	Rivanna				
> 45550185	ood_jupyter	b142c	gordan	49:33:57	bl	Running	Rivanna				
> 4561167	ood_studio	j2nrm	bl_ssdsl	05:39:05	bl	Running	Rivanna				
> 45614891	ood_jupyter	yj0t	bl_ssdsl	01:51:17	bl	Running	Rivanna				
> 45614509	ood_jupyter	yu2bk	bl_ssdsl	03:31:39	bl	Running	Rivanna				
> 45553758	ood_jupyter	huzlwk	biocomplexity	47:05:00	bl	Running	Rivanna				
> 45595263	ood_jupyter	sse0nx	biocomplexity	122:51:59	bl	Running	Rivanna				
> 45547177	ood_jupyter	asw3xp	bl_nsaac	52:06:27	bl	Running	Rivanna				
> 45614824	ood_jupyter	zrlfdw	biocomplexity	02:22:21	bl	Running	Rivanna				
> 45609234	ood_studio	cpr9lw	biocomplexity	06:49:26	bl	Running	Rivanna				
> 45545142	ood_jupyter	svbrv	nsaac_covid19	52:49:19	bl	Running	Rivanna				
> 45544368	ood_jupyter	pg2b	nsaac_covid19	53:49:29	bl	Running	Rivanna				
> 45615313	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:24:18	bl-gpu	Completed	Rivanna				
> 45615306	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:21:35	bl-gpu	Completed	Rivanna				
> 45615292	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:21:36	bl-gpu	Completed	Rivanna				
> 45615299	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:23:54	bl-gpu	Completed	Rivanna				
> 45615340	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:12:34	bl-gpu	Completed	Rivanna				
> 45615353	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:07:36	bl-gpu	Completed	Rivanna				
> 45615346	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:08:19	bl-gpu	Completed	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.

Active Jobs											
Show	50	entries									
ID	Name	User	Account	Time Used	Queue	Status	Cluster				
> 45615313	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:24:18	bl-gpu	Completed	Rivanna				
> 45615306	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:21:35	bl-gpu	Completed	Rivanna				
> 45615292	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:21:36	bl-gpu	Completed	Rivanna				
> 45615299	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:23:54	bl-gpu	Completed	Rivanna				
> 45615340	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:12:34	bl-gpu	Completed	Rivanna				
> 45615353	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:07:36	bl-gpu	Completed	Rivanna				
> 45615346	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:08:19	bl-gpu	Completed	Rivanna				
> 45612331	ood_jupyter	y1kdt	da7003-fel22	00:00:00	bl-gpu	Completed	Rivanna				
> 45615290	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:26:09	bl-gpu	Running	Rivanna				
> 45615341	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:14:20	bl-gpu	Running	Rivanna				
> 45615334	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:16:59	bl-gpu	Running	Rivanna				
> 45615327	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:20:02	bl-gpu	Running	Rivanna				
> 45615320	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:22:04	bl-gpu	Running	Rivanna				
> 45615318	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:23:11	bl-gpu	Running	Rivanna				
> 45615355	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:09:28	bl-gpu	Running	Rivanna				
> 45615344	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:09:48	bl-gpu	Running	Rivanna				
> 45615347	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	00:11:56	bl-gpu	Running	Rivanna				
> 45615348	run_proc_gpu_WM.batch	hnt9zt	biocomplexity	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.

Active Jobs											
Show	50	entries									
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				

Showing 1 to 2 of 2 entries

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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.

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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# Accessing a Terminal from Open OnDemand

A graphical user interface is useful, but on a system like Rivanna, eventually we must learn a little about the command line. Open OnDemand provides a simple terminal application.

[Clusters->\\_Rivanna Shell Access](#) opens a tab with a terminal application running.



Accessing a Rivanna shell from Open OnDemand.

You should be automatically logged in to a Rivanna frontend.

A simple shell window.

A limitation of the Open OnDemand shell is that you cannot run graphical applications through it. If you need to start a program with a graphical user interface, use FastX.

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# Exercise 2

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 stop the interactive job.

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When you log in to Rivanna, whether through Open OnDemand, FastX, or a command-line ssh, you are on one of the *login nodes* or *frontends*. Use of the frontend is restricted to short “housekeeping” tasks such as

- Writing your programs or scripts
- Compiling programs
- Submitting jobs
- You may run *very short* test runs with a limited number of cores and amount of memory. Your process will be terminated if it exceeds the time or memory limit.
- You may *not* run multiple processes at once, nor may you run production jobs.

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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**

You are limited to 350,000 files in your scratch directory.

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. This provides protection against accidental removal of a file, or rolling back an error to the previous version.

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# Checking Your Storage

To check how much disk space you have used in your home and scratch directories, open a Terminal through Open OnDemand or FastX, and type **hdquota** at the command-line prompt:

hdquota							
Type	Location	Name	Size	Used	Avail	Use%	
home	/home	mst3k	50G	35G	16G	69%	
Scratch usage for mst3k							
Block Limits							
Filesystem	Fileset	days	GB	quota	limit	in_doubt	grace
gpfs0	scratch	90	266	10240	12288	1	none

The **hdquota** command will also show usage for any research project or research standard storage to which you have access.

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# Software Modules

Many application software packages are installed on Rivanna, frequently in multiple versions. Software *modules* make it much easier for users to access the packages and versions they want to use. A *module* is a script provided by the system that sets up paths and any environment variables that may be needed in order to run the program(s).

## Module Commands

These must be typed into a terminal. The commands must be typed into each terminal window, before any other commands to use the software.

- List all available modules and versions.

```
module avail
```

- Show all available modules

```
module spider
```

- Show available modules for a specific package

```
module spider package
```

- Show modules with the in the description

```
module key <keyword>
```

- Load the module to set up the environment for the default version of some software.

```
module load <name>
```

Unless otherwise noted, the default version of a package will be that with the *highest* number. If a different version is default, a (D) will be printed next to its name.

- Load a specific version N.m of software mypackage.

```
module load package/N.m
```

- Swap one version for another

```
module swap mypackage/N.m mypackage/K.1
```

- List modules currently loaded in your environment.

```
module list
```

- Clear all modules

```
module purge
```

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# Using Modules

Find all available versions of MATLAB. You may see a different list.

```
module spider matlab
```

```
-----
```

```
matlab:
```

```
-----
```

Versions:  
matlab/R2017a  
matlab/R2020a  
matlab/R2020b  
matlab/R2021a  
matlab/R2021b  
matlab/R2022a  
matlab/R2022b

```
-----
```

For detailed information about a specific "matlab" package (including how to load the modu

Note that names that have a trailing (E) are extensions provided by other modules.

For example:

```
$ module spider matlab/R2022b
```

Load a specific version of MATLAB

```
module load matlab/R2022a
```

Change versions

```
module swap matlab/R2022a matlab/R022b
```

Clean up

```
module purge
```

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# Module Hierarchies

The module system is *hierarchical*. It may be necessary to load other modules in order to load a package. This can occur when different packages are created with different toolchains. The hierarchy prevents incompatible versions of libraries and applications from conflicting.

## Example: R

```
module spider R

-----
R:

Description:
  R is a free software environment for statistical computing and
  graphics.

Versions:
  R/3.5.3
  R/3.6.3
  R/4.0.3
  R/4.1.1
  R/4.2.1

Other possible modules matches:
  agrep  amber  amptorch  apr  apr-util  archspec  aria2  armadillo  ...
```

To find other possible module matches execute:

```
$ module -r spider '.*R.*'
```

For detailed information about a specific "R" package (including how to load the modules) use the module's full name.

Note that names that have a trailing (E) are extensions provided by other modules.

For example:

```
$ module spider R/4.2.1
```

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# Selecting A Module Version

After listing the available versions, we decide we want to use R version 4.0.3

```
module spider R/4.0.3
-----
R: R/4.0.3
-----
Description:
R is a free software environment for statistical computing and
graphics.
```

You will need to load all module(s) on any one of the lines below before the "R/4.0.3" module is available to load.

```
gcc/7.1.0  openmpi/3.1.4
intel/18.0  intelmpi/18.0
```

Help:

```
Description
=====
R is a free software environment for statistical computing and graphics.
```

```
More information
=====
- Homepage: http://www.r-project.org/
```

```
Included extensions
=====
assertthat-0.2.1, b-a, base64enc-0.1-3, cli-2.0.2, crayon-1.3.4, d-a,
digest-0.6.25, ellipsis-0.3.0, evaluate-0.14, fansi-0.4.1, float-0.2-4, g-
r,
g-r, glue-1.4.0, htmltools-0.4.0, IRdisplay-0.7.0, IRkernel-1.1,
jsonlite-1.6.1, m-e, pbzMQ-0.3-3, pillar-1.4.4, Rcpp-1.0.4.6, repr-1.1.0,
rlang-0.4.6, rlecuyer-0.3-5, s-p, s-t, s-t, t-o, u-t, utf8-1.1.4, uuid-0.1
-4,
vctrs-0.3.0
```

 Note the line "You will need to load all module(s) on any one of the lines below..." You should load *either* one set *or* the other, not both.

```
module load gcc/7.1.0
module load openmpi/3.1.4
module load R/4.0.3
```

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# Exercise 3

Log in to Rivanna through the Open OnDemand portal. Examine the menus. Starting from the Interactive Apps menu, log in to FastX (VPN required). Once on the desktop, click the square black icon in the ribbon in the upper left to start a Terminal window; alternatively, go the menu Applications->System Tools and click on MATE Terminal. In the terminal, list all **matlab** modules. Choose a version and load the module. Check which module you have loaded. Purge the module.

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# The Slurm Resource Manager

Interactive Apps in Open OnDemand are convenient but have limitations. For long jobs they may be inconvenient and sometimes unrealistic. In other cases, we may wish to submit many jobs at once, which is awkward with interactive work. Finally, if we are running Jupyter notebooks, a network interruption could kill the process we are trying to run. For all of these cases, the solution is to run *batch* jobs. They will run in the background and you can return later to get the output.

To run batch jobs, a user logs in to one of the frontends, or to Open OnDemand. A *job request* is prepared for the compute nodes. The job request contains all the information required to request resources (cores, memory, GPU hardware, and so forth) and the instructions for carrying out the computation. For batch runs, this request takes the form of a *job script*, which is usually a specialized form of a *bash* script. The script is then submitted to the Slurm system.

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# The Open OnDemand Job Composer

You can use the OOD Job Composer to construct a job script and submit the job. Start by selecting a template script, which usually must be edited for customization to your job requirements. We can run the demo script with only minor changes so let us start there. From Job Composer choose New Job, From Default Template.

Jobs

Create a new job from the default template

From Default Template

From Template

From Specified Path

From Selected Job

Created

Name

ID

Cluster

Status

Search:

Default template

Job was successfully destroyed.

At the bottom left, click the “Open Editor” button. Change `your_allocation` to your allocation group name. Click the Save button at the upper left. Back in the Job Composer, refresh the page and make sure your change has taken effect. Click the green “Submit” button. The job status will be shown. Once it has changed to Completed, note that the Folder Contents section contains a new file. This will be named something like `slurm-123456.out` where the actual number corresponds to the job ID of your job. This will contain the output of your job.

Jobs

+ New Job

Edit Files

Job Options

Open Terminal

Submit

Stop

Show 25 entries

Created

Name

ID

Cluster

Status

Search:

January 10, 2023 3:25pm

demo\_hello\_world

45937679

Rivanna

Completed

Job was successfully submitted.

Job completion.

Click on the slurm file and it should open in the editor. Alternatively, click on “Open Dir” to open the File Explorer in the directory from which OOD ran your job, where you may View or Edit any of the files.

## Canceling a Job

This job will run so quickly you will probably not be able to stop it before it completes, but for other jobs that run longer, if you need to cancel the job, click the yellow “Stop” button. Do not use Delete for this purpose.

## Deleting a Job

"Deleting" a job removes the files from the directory specified in the "Script Location" entry. This helps you clean up your home directory. You may also do this manually through the File Explorer or on FastX. You may choose to create a directory with a more descriptive name than the OOD default and move your files there.

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# The Slurm Script

The “Hello World” demo Slurm script contains the information required to request resources and run the job.

```
#!/bin/bash

#SBATCH --ntasks=1
#SBATCH --mem=6000
#SBATCH --partition=standard
#SBATCH --account=your_allocation
#SBATCH --time=00:10:00

echo "Hello $USER, this is node $(hostname)."
```

Let's look at this script line by line.

```
#!/bin/bash
```

This tells the system that the file is a *bash script*. Bash is the default *shell* on Linux. A shell is a program that sits between the user and the operating system and enables us to interact with the system. When you use a terminal to type commands, you are probably using bash. But bash is also a programming language and we can write scripts for it.

```
#SBATCH --ntasks=1
```

This is a resource request. Every request starts with the string

```
#SBATCH
```

Here we are requesting one *task* (ntasks stands for number of tasks). To Slurm, a task is a process carried out by the operating system. Most usually, it is your program's executable. In this case, we are asking for a single process on a single core.

```
#SBATCH --mem=6000
```

This requests a total of 6000MB or 6GB of memory. This is for the total amount of memory over the entire set of cores to be used, so typically the request would be larger, or we would use another form

```
#SBATCH --mem-per-cpu=9000
```

This stands for “memory per cpu” (Slurm still often refers to a core as a “cpu”).

```
#SBATCH --partition=standard
```

This requests the partition to which the job will be submitted.

```
#SBATCH --account=your_allocation
```

Specifies the allocation to be charged. (This does not refer to your user account.)

```
#SBATCH --time=00:10:00
```

Request that the job should run for 10 minutes. It is a good idea to try to get an accurate estimate of the time you will need for the job, in order not to use SUs unnecessarily.

```
echo "Hello $USER, this is node $(hostname)."
```

This line executes the job. It is a command to bash to print a string. Your user ID is substituted for \$USER, and the node on which it's running for hostname.

When you submit the job, a process called the *scheduler* examines your script, looking at all lines starting with #SBATCH. It extracts the resources requested and places your job in the appropriate partition.

Once your job starts, the script is executed on the compute node as a normal bash script. In bash scripts, lines that begin with the hash symbol `#` are comments and are ignored.

There are many other options for Slurm. See our [documentation](#) or the developer's [cheat sheet](#). The templates available through OOD also provide more examples.

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# Slurm Partitions

To see a list of available partitions, from a terminal type

qlist

Queue (partition)	Total Cores	Free Cores	Jobs Running	Jobs Pending	Time Limit	SU Charge
<hr/>						
bii	4640	4335	18	3	7-00:00:00	1
standard	5644	3249		672	7-00:00:00	1
dev	456	428			1:00:00	0
parallel	5760	1056	37	2	3-00:00:00	1
instructional	2320	839		1	3-00:00:00	1
largemem	208	154	13	1	4-00:00:00	1
gpu	2052	1258		61	3-00:00:00	3
bii-gpu	608	367	16	1	3-00:00:00	1
bii-largemem	288	248		2	7-00:00:00	1

The resources available in each partition are as follows. Rivanna is a heterogeneous system, so available cores and memory may vary within one partition.

Queue Name	Purpose	Job Time Limit	Memory / Node	Cores / Node
standard	For jobs on a single compute node	7 days	256 GB/384 GB/768 GB	28/40/40
gpu	For jobs that can use general purpose graphical processing units (GPGPUs)/(K80, P100, V100)	3 days	256 GB/384 GB/1 TB	28/40/128
parallel	For large parallel jobs on up to 25 nodes (<=1000 cores over all jobs)	3 days	384 GB	40
largemem	For memory intensive jobs (<=16 cores/node)	4 days	1 TB	16
dev	To run jobs that are quick tests of code (<=2 nodes, 8 cores/node)	1 hour	128 GB	4

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# Using a Template

The default demo Slurm script template is very simple and it would be easier to start from something closer to your intentions. We provide quite a few sample script templates.



The example shown here is from a particular time and the templates may be updated. What you see may not be the same as in these illustrations, but the steps to follow should be the same.

Suppose we wish to run a serial (one core) Python program. From New Job we select From Template. We can search on the string `python` to narrow the options. We find `demo-python-serial`. Select that option. Click “Create New Job” to make the folder and copy the demo files into it.

**Templates**  
To create a new job, select a template to copy, fill out the form to the right, and click “Create New Job”.

The screenshot shows a table of templates with columns for Name, Cluster, and Source. A search bar at the top right is set to "python". To the right, a "Create New" dialog is open for "demo-python-serial" with fields for Job Name, Cluster, and Script Name, and a "Create New Job" button.

Select the template you wish to use.

As before, edit the Slurm script to fill in your correct allocation group name. Also make sure the module loaded is just `anaconda`.

```
module purge
module load anaconda
```

## Templates

To create a new job, select a template to copy, fill out the form to the right, and click “Create New Job”.

The screenshot shows a table of templates with columns for Name, Cluster, and Source. A search bar at the top right is set to "python". To the right, a "Create New" dialog is open for "demo-python-serial" with fields for Job Name, Cluster, and Script Name, and a "Create New Job" button.

Select the template you wish to use.

Submit the job. Once it returns, look at the output. Oops!

```
File "hello.py", line 6
    print "\n %5d  Hello World!" % (i+1)
               ^
SyntaxError: invalid syntax
```

Select the template you wish to use.

An error occurred. In a real job, your output should have been what you expected, and you can proceed as for the default demo example to manage your result files.

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# Using a Script from a Path or Job

We had a syntax error in our Python script. After looking at it, we realize that our Python script is written for Python 2, but the `anaconda` module loads Python 3. We open a terminal and type

```
module spider anaconda
```

## From a Path

```
$module spider anaconda
.
.
.
anaconda:
Description: Built to complement the rich, open source Python community, the Anaconda platform provides an enterprise-ready data analytics platform that empowers companies to adopt a modern open data science analytics architecture.
Versions:
  anaconda/2019.10-py2.7
  anaconda/2020.11-py3.8

For detailed information about a specific "anaconda" package (including how to load the modules) use the module's full name.
Note that names that have a trailing (c) are extensions provided by other modules.
For example:
$ module spider anaconda/2020.11-py3.8
```

Result from checking versions of anaconda.

The default is

```
anaconda/2020.11-py3.8
```

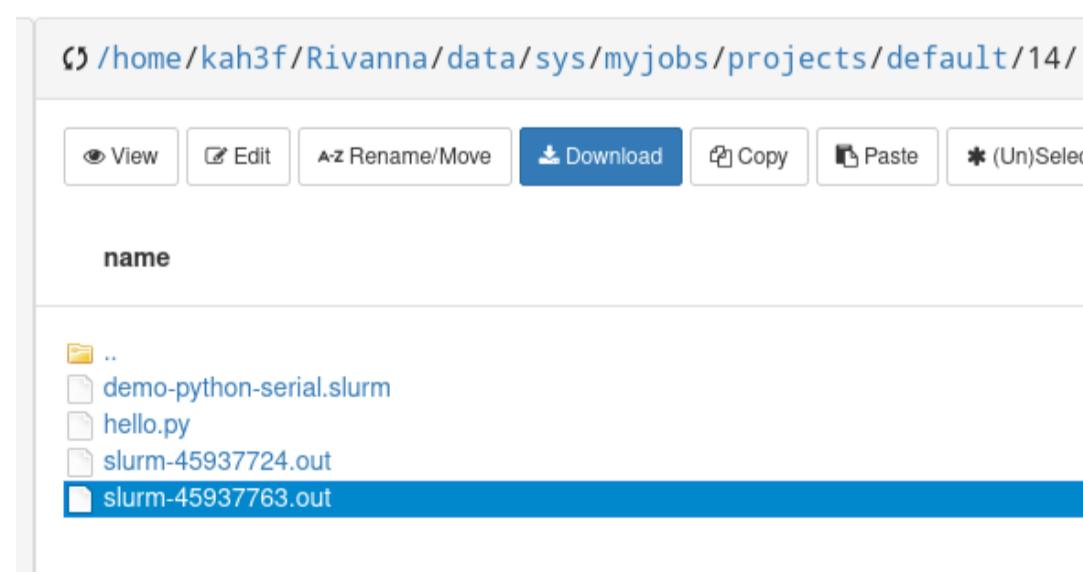
We need to use

```
anaconda/2019.10-py2.7
```

We have most of the files we need in the failed job's folder, so we can start a new job from the path to that folder and they will be copied.

Select the path to the job and copy it to your clipboard. From the “New Job” dropdown, choose “From Specified Path.” When the form opens, paste in the path. It will complain that the script name is missing, but you can open Job Options as it requests, and generally it will find the correct script to copy. You will then be able to edit it as before to change the module. Submit the job.

When it completes, go to the directory. Note that it copied all the files, including the Slurm output from the failed job.



Corrected job (we hope).

View the `slurm-123456.out` file. You should see

```
1 Hello World!  
2 Hello World!  
3 Hello World!  
4 Hello World!  
5 Hello World!  
6 Hello World!  
7 Hello World!  
8 Hello World!  
9 Hello World!  
10 Hello World!
```

Result from the correct version of anaconda.

## From Another Job

The New Job option “From Selected Job” is similar, but can only be used with existing jobs, whereas “From a Path” could copy from a master path to new jobs. From Selected Job should be self-explanatory once you understand the Path option.

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# Preparing and Submitting from the Command Line

Users who are comfortable with the command line can submit jobs directly. This is currently necessary in order to run jobs from /scratch or /project.

For a more in-depth introduction to using Rivanna from a command line, see our [tutorial](#).

## Prepare a Folder

Most of the time, it is advisable for you to have a folder for each job or set of related jobs.

You can use OOD's File Explorer to set up your directories if you are not yet comfortable using a command line. This folder should contain all the files you need to run your job.

## Write the Script

You must first write a script. You may use an OOD template, or one of our [examples](#). If you know a text editor you can use that to edit the template. Otherwise you can use the built-in OOD text editor, or you can use pluma/gedit through FastX. Please do not use LibreOffice. Slurm scripts should not be created or edited on your local computer; always use a Rivanna frontend.

Slurm's default is to change into the folder from which the job was submitted, so make sure your script is where you intend the job to run.

## Submit the Script

You must navigate to the directory you created. Suppose it is `/scratch/mst3k/myjob`. From a terminal, use the `cd` (change directory) command.

```
cd /scratch/mst3k/myjob
```

Now you can submit the script with the `sbatch` command.

```
sbatch myscript.slurm
```

The system will return the *job id*

```
Submitted batch job 123456
```

To use a directory in leased /project storage, substitute the appropriate path, starting with /project, for the scratch directory. Otherwise the process is the same.

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# Checking Jobs from the Command Line

Regardless of how the job was submitted, through the Job Composer or at a command line, you can use the Open OnDemand Job Viewer or you can use command-line tools to monitor your job.

If you are using a terminal you can type

```
squeue
```

to view all jobs, and

```
squeue -u mst3k
```

with your user ID, to view only your jobs. To view a specific queue

```
squeue -p partition
```

Information about a running job, use `sacct` with the job ID.

```
sacct -j 12345
```

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# Using More Than One Core

Every example we have considered so far was a *serial* job, i.e. it ran on a single core on a single node. However, much of the benefit of a high-performance cluster like Rivanna is the ability to utilize many cores at once. This is called *parallelism*.

## High-Throughput Parallelism

In high-throughput parallelism, each job runs on a single core (or perhaps a small number of cores) but we want to run many of them, up to hundreds or thousands. Most high-throughput workflows can be set up as a *job array*. Please see our [example](#). When submitted, a job array receives a Slurm job ID as usual, but each subtask also has an “array task ID” associated with it. The  `${SLURM_ARRAY_TASK_ID}` is an *environment variable*. It is assigned by Slurm when the job is initiated. You can use it in your scripts but should not attempt to set its value. It will take on the array task ID for each subtask when it is started. The job script for each array task is identical; variables allow for different patterns in input/output files and such.

Job arrays should be submitted to the standard partition, unless individual array tasks can use multiple nodes. You may submit more array tasks than are allowed to run at one time; currently the limit is 9999. Slurm will start as many as possible initially, then as an array task completes, the next in line will be started.

The OOD Job Composer has several job-array templates (search on “array”). You can copy them without submitting a job, and modify them for your needs.

## Multicore, Single Node

Some programs are able to run on more than one core but must be kept on the same node. This is *threading*. Our example script is [here](#). You should find out how your program or script sets the number of threads; typically this is by some environment variable like  `$NTHREADS`. That should be set to  `` ${SLURM_CPUS_PER_TASK}`` in your script. The corresponding resource requests are

```
$SBATCH --ntasks=1  
$SBATCH --cpus-per-task=8
```

The `--cpus-per-task` option can also be abbreviated

```
$SBATCH -c 8
```

Using this request will ensure that cores for the threads for each controlling task will be on the same node.

Keep in mind that a program must be written for threading; it does not happen automatically.

Threaded programs must use the standard partition.

## Multicore, Multinode

Some programs can utilize not only more than one core, but more than one node. Most of these programs use the Message Passing Interface (MPI). An example script is [available](#). In this type of program, each process runs independently and communicates with the others. Slurm regards each of these processes as a separate task, so the requests are

```
$SBATCH --nodes=2  
$SBATCH --ntasks-per-node=40
```

This example will run a total of 80 processes. The Slurm `srun` command should be used to launch the tasks.

Distributed programs may use the standard partition if running on a single node. The parallel partition is available for jobs using more than one node.

## GPUs

GPUs must be requested explicitly as a resource. This is accomplished through a `gres` (generic resource) and the job must be submitted to the gpu partition. The architecture may be specified. More information is available [here](#).

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# **Exercise 4**

Follow along with the notes to run the OOD Job Composer demo ("Hello World") job.

## **Bonus 1**

Choose a template closer to what you intend to run. Modify the script file appropriately. Run the job.

## **Bonus 2**

Using the File Explorer or Caja (or the command line), make a directory. Copy a template script file to that directory. Edit the file appropriately. Submit the job from the command line.

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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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