FH Cluster Guide

September 22, 2022

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About this Course

Our goal is to get you running on the Fred Hutch cluster quickly and efficiently with this quick-start guide. As a wise Drivers' Ed instructor once said, **you need to go slow to go fast!**

In this short course, you'll invest a bit of time now to save you time and frustration down the road. Follow along at **any time on your own schedule**. We hope that the following modules will help you take advantage of the powerful resources the Fred Hutch has to offer!

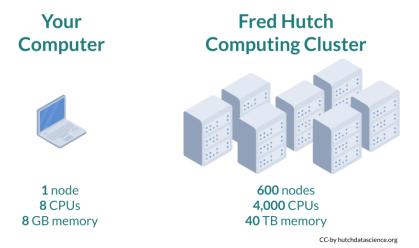
6 CONTENTS

Cluster 101

What is a Cluster?

A computing cluster is a set of many computers networked together. Because there are many computers working together, the network is able to handle computationally expensive tasks, like genome assemblies or advanced algorithms. Imagine you're building a house. It would take a long time by yourself! It's much better to have many builders working together.

Now that we have a team of workers, the next challenge is task management. A home construction team will need a manager to help delegate tasks. Similarly, the computing cluster uses management software to prioritize tasks, delegate workers (resources), and check on progress. The Fred Hutch cluster uses a common management and scheduling tool called Slurm.



How is the cluster different from a laptop or desktop? First, you might use an operating system like Windows or MacOS. The Fred Hutch server is a Linux

system. Second, because many people use the cluster for many tasks, there isn't a central screen and keyboard. You access the cluster remotely from your computer! We will talk more about how to connect to the cluster in a following chapter.

Computing cluster

A set of computers networked together to perform large tasks.

Account Setup

You will need an account to log in to the cluster. This ensures that data stays protected.

2.1 Check your HutchNet ID

Your HutchNet ID is the standard login you receive when you start working at the Hutch or are an official affiliate. You can use it to login to most resources at the Center (Desktop Computer, Employee Self Service, VPN, Webmail) and our Scientific Computing systems.

For example:

- my email is jsmith3@fredhutch.org.
- my HutchNet ID is jsmith3.

If one of your collaborators requires access to the Fred Hutch network you can submit a non-employee action form. Non-employee is a generic administrative term for affiliates, students, contractors, etc.

2.2 Contacting the SciComp Team

To use Scientific Computing clusters at Hutch, your HutchNet ID must be associated with a PI account.

The Scientific Computing Team (SciComp) tries to set some users up ahead of time. However, not everyone is set up automatically. Please fill out this Account Setup Form and we will ensure you are set up correctly!

Errors similar to "Invalid account or account/partition" typically indicate that the account hasn't been set up by SciComp. This is a quick fix if you use the form above.

Now, let's set up our Terminal!

Terminal Setup

The next step is getting familiar with your Terminal. This is your portal to the cluster.

3.1 What is a terminal?

The Terminal is a command line interface. In other words, the Terminal is a software application that allows you to issue commands directly to your laptop or desktop computer. The Terminal is very useful because it allows you to run commands that don't have a graphical user interface (GUI). It can also connect you to computer networks, such as the Fred Hutch cluster! The Terminal setup is different depending on your operating system. Jump to the Windows, MacOS, or Linux sections below.

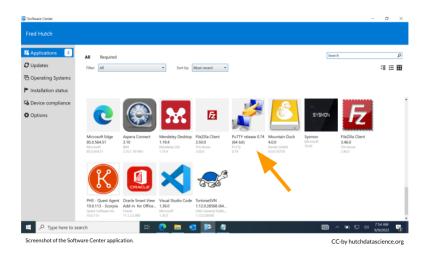
"Terminal" used to be synonymous with "computer". With the creation of operating systems like Windows and MacOS, computers became much easier to use and exploded in popularity! Your colleagues are almost always referring to the command line application when they say "Terminal".

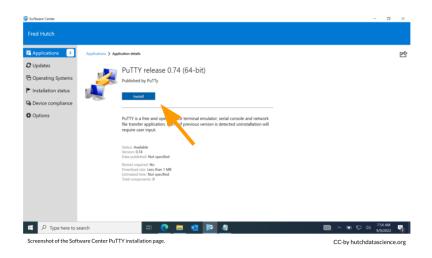
3.2 Windows Setup

Click to view steps

You will need to install a Terminal application called PuTTY to connect to the Fred Hutch Cluster.

1. You should then see PuTTY available in the Software Center. Click "Install" and go through the Setup Wizard.





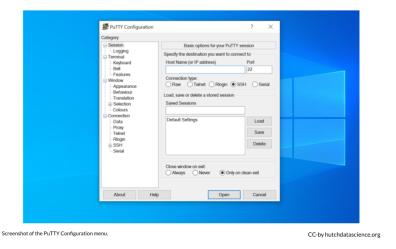
You can also install PuTTY manually if you don't see it in the Software Center.

2. PuTTY should now be available in your applications. Click on PuTTY to open.

3.3. MAC SETUP 15



3. You should now see the PuTTY Configuration menu.

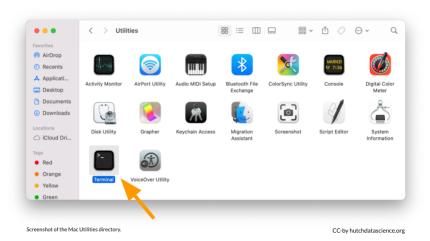


3.3 Mac Setup

Click to view steps

Mac machines come with a Terminal installed.

1. Go to Finder > Applications > Utilities > Terminal and double-click.



2. Your Terminal should look like this:



3.4 Linux Setup

Click to view steps

The commonly used Linux distribution, Ubuntu, already comes with a Terminal installed.

1. Press ctrl + alt + T. Your open Terminal window should look like this:

[SCREENSHOT]

1. Update the Terminal and prepare it for connecting to the cluster by running:

sudo apt install openssh-server

Enter your password and enter Y when prompted.

Logging In

Now that you have your Terminal application ready, you want to connect to the cluster. You will do this using a method called SSH, which stands for "Secure SHell".

4.1 What is SSH?

SSH is a secure way to remotely connect to another computer or network of computers. In other words, SSH helps us protect your data and the data on the Fred Hutch cluster through authentication.

Hostname

The hostname is the name, or label, assigned to a computer in a network. We are connecting to hostname rhino.fhcrc.org or rhino for short.

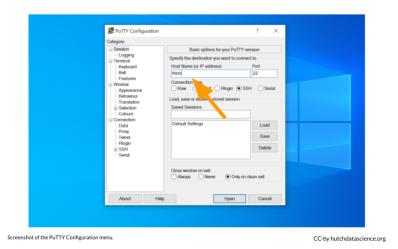
Before moving on, you will need to connect to the Fred Hutch wifi network, a networked ethernet jack, or the Fred Hutch VPN. This is the first layer of security.

The next set of steps are specific to your operating system.

4.2 Windows Login

Click to view steps

1. Go to the PuTTY Configuration menu. Under "Host Name" type **rhino** and click "Open".

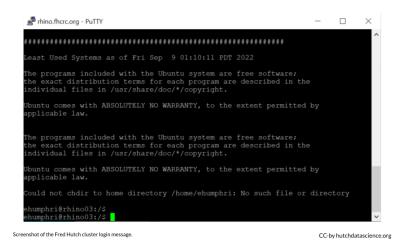


2. You will be prompted to login. Type in your HutchNetID (e.g., jsmith3).



- 3. Enter your password. No* or symbols will show up, so type it in carefully!
- $4.\,$ You are now logged in! There should be a login message, with your name at the bottom.

4.3. MAC LOGIN 21



Congratulations! You are now logged in to the Fred Hutch cluster!

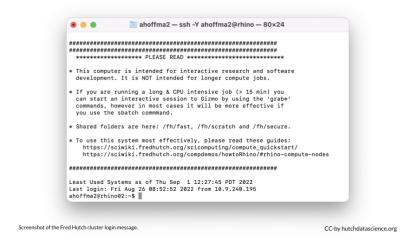
4.3 Mac Login

Click to view steps

1. Type the following commands, substituting in your HutchNet ID:

```
ssh -Y HutchID@rhino
```

- 2. You will see a message that looks like The authenticity of host 'rhino (XXX.XXX.XX)' can't be established. Type in yes and hit enter.
- 3. Enter your password. No* or symbols will show up, so type it in carefully!
- 4. You are now logged in! There should be a login message, with your name at the bottom.



Congratulations! You are now logged in to the Fred Hutch cluster!

4.4 Linux Login

Click to view steps

Congratulations! You are now logged in to the Fred Hutch cluster!

Submit your first job

The Fred Hutch cluster uses Slurm to organize and prioritize jobs. Instead of running commands directly on rhino, you will submit a script (a snippet of directions) to tell Slurm what to do.

5.1 Download the script

We can use the wget command to download a script from GitHub. This means we don't have to write the script from scratch. Copy and paste the following into the terminal, and hit return:

wget https://raw.githubusercontent.com/FredHutch/slurm-examples/master/introduction/1-hello-world



5.2 Confirm the download

Let's confirm that we can see the file we just downloaded. We can use the 1s (list files) command for this. Type 1s and hit return. You should see the file 01.sh in your home directory. The .sh ending means this is a script meant to run from the command line.

ls



5.3 Inspect the script

Let's next inspect the script. The cat command, followed by a file name, lists the entire contents of a specific file.

cat 01.sh



- The first line of the script, #!/bin/bash, indicates that this is a command line or "bash" script.
- The second line is empty, and the third line, echo "Hello, World" means that the computer will "echo", or print out, "Hello, World".

5.4 Submit the script

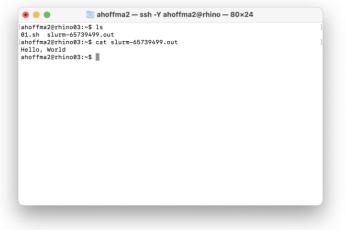
We use the sbatch command to submit a script and start running a job on the cluster. Copy the following and hit return. You should see a message like "Submitted batch job 12345678". Your number will vary because this is a unique job identifier.

sbatch 01.sh

5.5 Check the output

Type 1s again. You should now see a log file like slurm-12345678.out listed alongside your script 01.sh. Let's use cat to inspect the output in the log file. We should see our message has been printed!

cat slurm-<your-number-here>.out



Screenshot of cat command output, the contents of the log file.

CC-by hutchdatascience.org

ls

This command lists the files in the current directory.

 $\mathtt{cat}\ \mathit{filename}$

This command prints the contents of a specific file .

 $\mathtt{sbatch}\ filename.sh$

This command submits a job to the cluster with instructions specified in .sh

File upload and download

Exchanging files with the cluster is very important. You can imagine scenarios where:

- You want to download log files or output files
- You want to upload a custom .sh script file that you wrote on your laptop
- You want to upload other files

In this course, upload and download of files is performed using Cyberduck. Cyberduck is a tool that lets us connect to the cluster securely, browse files, and transfer files securely.

6.1 Download Cyberduck

Download the latest version of Cyberduck here.

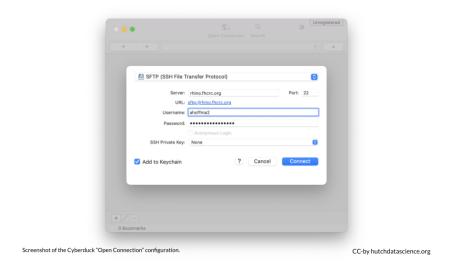
Note that the version of Cyberduck in the Software Center or Self Service might not be current, causing compatibility issues with some operating systems.

6.2 Create Connection

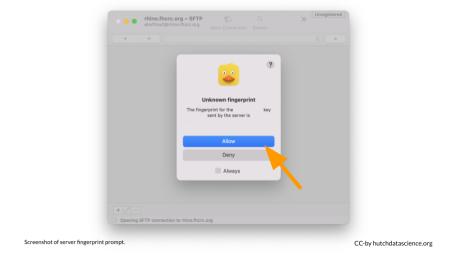
Launch Cyberduck and click on "Open Connection".

- From the dropdown menu, select "SFTP (SSH File Transfer Protocol)"
- For Server, type "rhino.fhcrc.org"
- Fill in your HutchNetID for Username and fill in your password

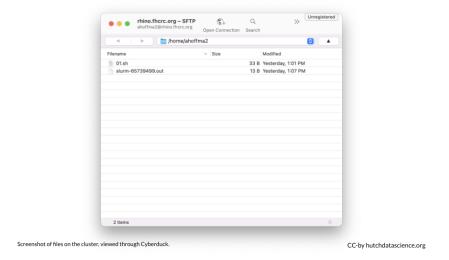
Click "Connect"



Click "Allow". You can also check the box to indicate "Always".

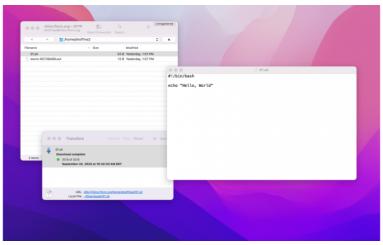


You should see your script file "01.sh" and the log file.



6.3 Download and edit the script

- Right click on "01.sh" and select "Download"
- You will see a "Transfers" prompt open, and the O1.sh file should now appear in your Downloads folder
- Open the 01.sh file



Screenshot of files, Transfers window, and the downloaded script.

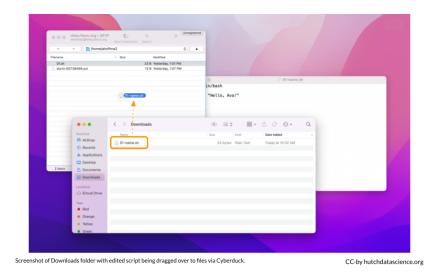
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Edit the message to include your name and save the file. Rename the file 01-name.sh

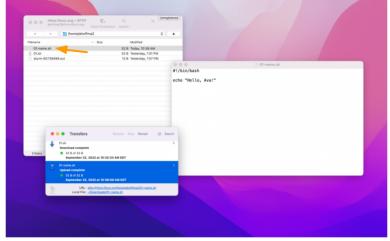


6.4 Upload the new script

From your Downloads folder, simply drag the file to Cyberduck.



You should now see the new script among your cluster files.



 ${\it Screenshot}\ of\ edited\ script\ among\ cluster\ files\ visible\ on\ Cyberduck.$

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6.5 Run the new script

Return to your Terminal. Submit a job with your new script by running the following. When you type 1s you should see a new log file!

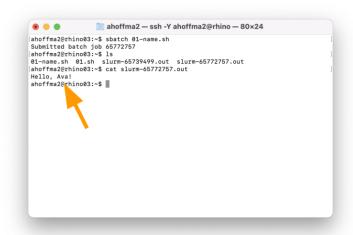
sbatch 01-name.sh



The job numbers included in log file names generally increase in number. The greater the number, the more recently the job was run.

Use the cat command to inspect the log. The message should show the new text that you added!

cat slurm-<your-number-here>.out



Screenshot of edited script message output using 'cat' command

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Interactive cluster

Assessment

Cluster 101 Self Test

Appendix

Where to get help

We want to help! Here are some ways you can get help for your work on the cluster.

Submit a Ticket

Submitting a good ticket helps the SciComp Team address your needs quickly and efficiently. We suggest you submit the following in a ticket:

- 1.
- 2.
- 3.

Visit the SciWiki

The SciWiki Scientific Computing page is full of useful tips and guides.

Provide Feedback

Please submit an issue at our GitHub repository. You can also click the edit button on the top of the page in question.

FAQ / Troubleshooting

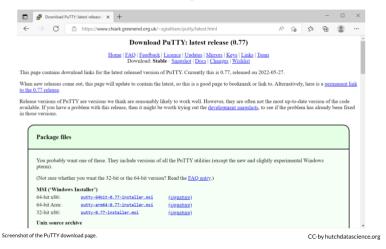
11.1 FAQ

Here are some questions you might have.

11.1.1 How can I manually install PuTTY?

Click to view steps

1. Click here to install the latest version of PuTTY. You will choose the 64-bit x86 installation with few exceptions.



2. Click through to install via the Setup Wizard.

11.2 Troubleshooting

Here are some issues you might encounter.

ssh: Could not resolve hostname rhino: nodename nor servname provided, or not known

Click to view steps

This error means that your computer is having trouble connecting to rhino. Ensure one of the following is true:

- 1. You are connected to the Fred Hutch wifi network on campus.
- 2. You are connected to the Fred Hutch VPN
- 3. You are plugged into an ethernet cable on campus that taps into the Fred Hutch network. Note that not all ethernet wall jacks have this capability, so try another jack if you are having trouble. Please email the IT helpdesk and include your office number and the number on the jack if you find a jack that isn't working.

ssh: connect to host rhino port 22: Undefined error: 0

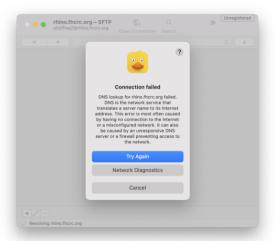
Click to view steps

This likely indicates a disruption to your internet connection and/or VPN. Ensure you are connected to the internet and connected to the Fred Hutch network on campus or the VPN.

Connection failed message in Cyberduck

Click to view steps

This likely indicates a disruption to your internet connection and/or VPN. Ensure you are connected to the internet and connected to the Fred Hutch network on campus or the VPN.



Screenshot of the Cyberduck "Connection failed" message.

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About the Authors

These credits are based on our course contributors table guidelines.

Credits	Names	
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make new line if more than one chapter		
involved		
Content Author(s) (include chapter	If any other authors besides	
name/link in parentheses if only for specific	lead instructor	
chapters) - make new line if more than one		
chapter involved Content Contributor(s) (include section	Wrote less than a chapter	
name/link in parentheses) - make new line	wrote less than a chapter	
if more than one section involved		
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Content Director(s)	Helped guide the content	
	direction	
Content Consultants (include chapter	Gave high level advice on	
name/link in parentheses or word	content	
"General") - make new line if more than		
one chapter involved		
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	content but not to the level of consulting	
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Contone 1 disherer(c)	platform	
Content Publishing Reviewer(s)	Reviewed overall content and	
. ,	aesthetics on publishing	
	platform	

Credits	Names
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Figure Artist(s)	Created figures/plots for course
Videographer(s)	Filmed videos
Videography Editor(s)	Edited film
Audiographer(s)	Recorded audio
Audiography Editor(s)	Edited audio recordings
Funding	
Funder(s)	Institution/individual who funded course including grant number
Funding Staff	Staff members who help with funding

[2] /usr/local/lib/R/library

```
##
   callr
                 3.4.4
                             2020-09-07 [1] RSPM (R 4.0.2)
##
                 2.0.2
                             2020-02-28 [1] RSPM (R 4.0.0)
   cli
##
                 1.3.4
                            2017-09-16 [1] RSPM (R 4.0.0)
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## desc
                 1.2.0
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##
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                 2.3.2
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##
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                 0.4.1
                            2020-01-08 [1] RSPM (R 4.0.0)
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##
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## magrittr
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                            2022-01-26 [1] CRAN (R 4.0.2)
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                 1.1.0
##
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## R6
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##
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## rprojroot
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                            2020-11-15 [1] CRAN (R 4.0.2)
                            2018-11-05 [1] RSPM (R 4.0.3)
##
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                 1.1.1
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                 1.5.3
                            2020-09-09 [1] RSPM (R 4.0.3)
## stringr
                 1.4.0
                            2019-02-10 [1] RSPM (R 4.0.3)
                             2022-02-15 [1] Github (R-lib/testthat@e99155a)
## testthat
                 3.0.1
                 2.1.5.9000 2022-02-15 [1] Github (r-lib/usethis@57b109a)
##
   usethis
## withr
                 2.3.0
                            2020-09-22 [1] RSPM (R 4.0.2)
## xfun
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                            2022-08-10 [1] CRAN (R 4.0.2)
                            2020-02-01 [1] RSPM (R 4.0.3)
##
   yaml
                 2.2.1
## [1] /usr/local/lib/R/site-library
```

References