Minerva HPC Computing Users' Guide

Overview

This guide will help you login and become familiar with running analyses on the Mount Sinai Minerva HPC servers.

Contents

Software Requirement to connect to Minerva

Mac/Linux

- Both Mac and Linux operating systems have built in terminal programs
- If you are going to be using GUIs (graphical user interfaces – like application windows), you will need to install a X11 server.
  - On Mac, we recommend use of **XQuartz**
  - On Linux, an X11 server should come preinstalled

Windows

- **Install MobaXterm** from https://mobaxterm.mobatek.net/
  - Enhanced terminal for Windows with X11 server, tabbed SSH client, network tools and much more

OR

- **Install PuTTY** from www.putty.org
  - If you are going to be using GUI's, in Putty: Connection > SSH > X11
  - Ensure "Enable X11 forwarding" is selected
  - On Windows box install Xming
  - Test by logging into Minerva and run the command: xclock
    - Should see a clock

OR

- **Install Windows Subsystem for Linux (WSL)** here
  - Run a Linux environment - including most command-line tools, utilities, and applications -- directly on Windows, unmodified, without the overhead of a traditional virtual machine or dual boot setup

Basic Linux Command Line Resources

https://www.digitalocean.com/community/tutorials/basic-linux-navigation-and-file-management

Navigating the Minerva Environment

Logging in

1. Connect to VPN, if off-campus

Before logging into Minerva, you must be connected to the Sinai network. If you are off-campus, that means you need to connect to run the **VPN Tunnel**. To access this log into msvpn.mssm.edu (School Users and all External Users), or vpn.mountsinai.org (Health System Users).

2. Logging in to Minerva via SSH

At your terminal program (xTerm, MobaXterm, puTTY) you will SSH (Secure Shell) into the Minerva platform.

ssh -Y *mssm_login_id*@minerva.hpc.mssm.edu

So, for example:

Assuming your userid is **lastnf03**

ssh -Y lastnf03@minerva.hpc.mssm.edu

3. Enter your Password

It will prompt you for a password:

Password: {your_MSSM_password}{your6digit-VIP-Access-VPN-key}

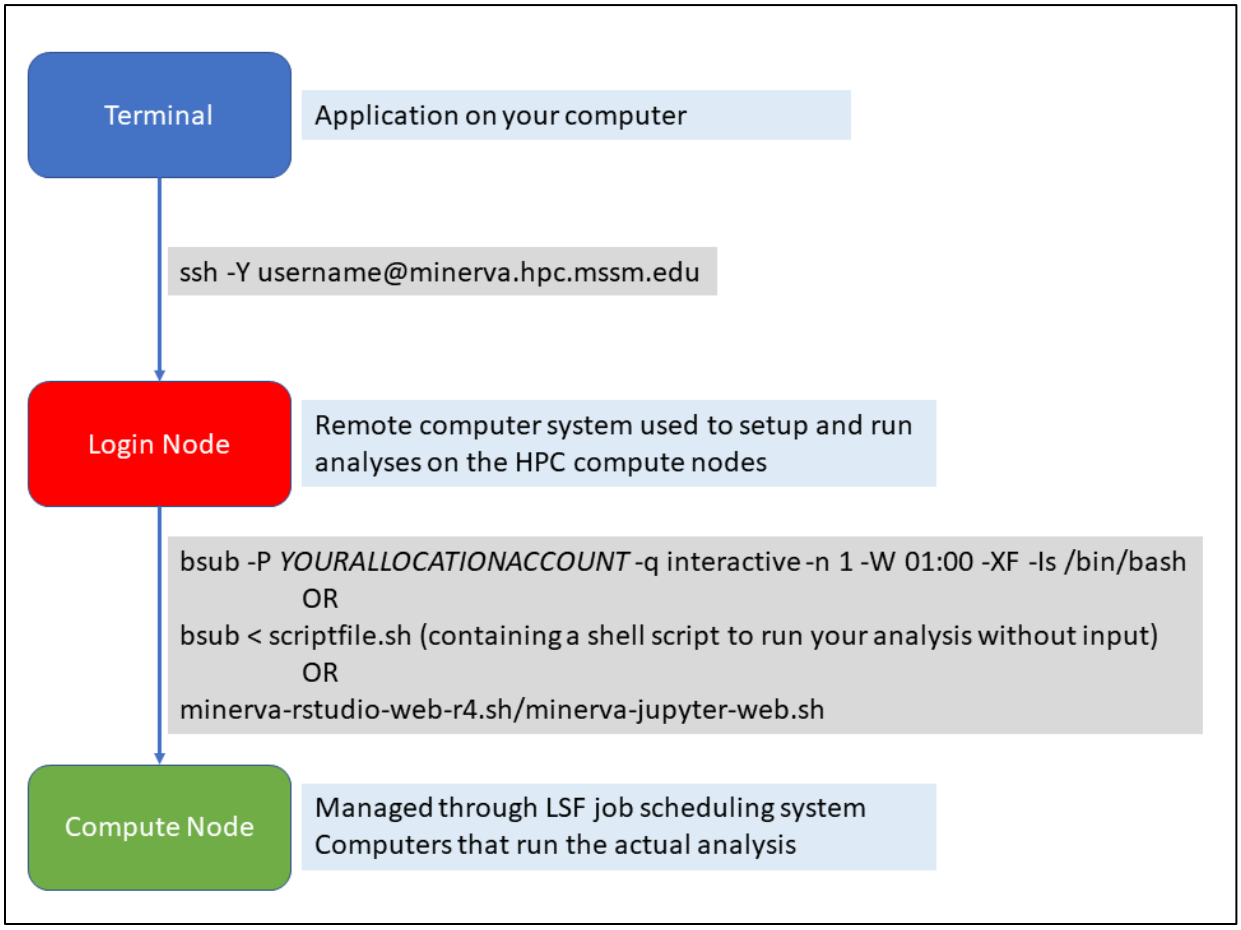
So, for example:

Assuming your MSSM password is **PassWord** and you VIP Access VPN Key (from the App on your phone) is 123456

Password: PassWord123456

If your account is locked or disabled, email hpchelp@hpc.mssm.edu and copy Alexis and Dave.

Minerva Connection Diagram



Login Nodes

When you first connect to Minerva, you will land on a login node at your home directory.

- Never run jobs directly on login nodes
- For file management, coding, compilation, check/manage jobs etc., purposes only
- Basic linux command: cd, ls and more

From the login nodes you will submit jobs to the LSF scheduler and/or start a interactive session of the server.

Compute Nodes

Compute nodes are where your scripted jobs and analysis are performed. You can not directly connect to a compute node, but interactive sessions, containerized applications (such as RStudio and Jupyter Notebook) and batch script jobs are run on these nodes.

General Minerva Storage information

- Storage is in folders and subfolders. In Linux, subfolders are separated by "/"
- 4 folders you can have (Possibly multiple project folders)
- Use showquota to show /sc/arion usage by user or project

  $ *showquota -u gail01 arion* or $ *showquota -p projectname arion*

Home	/hpc/users/<userid> $ **quota -s**	• 20GB quota. • Slow. Use for "config" files, executables…NOT DATA • NOT purged and is backed up
Work	/sc/arion/work/<userid> $ **df -h** /sc/arion/work<userid>	• 100GB quota • Fast, keep your personal data here • NOT purged but is NOT backed up
Scratch	/sc/arion/scratch/<userid> $ **df -h** /sc/arion/scratch	• Free for all, shared by all; For temporary data • Current size is about 100TB • Purge every 14 days and limit per user is 10TB
Project	/sc/arion/projects/<projectid> $ **df -h** /sc/arion/projects/<projectid>	• PI's can request project storage by submitting an allocation request at here,and get approval from allocation committee; Fee schedule and policy here • Not backed up • Incurs charges **$100**/TiB/yr

* The EMHSR team takes care of backing up our project folders on a regular basis.

Specific file structures within the EMHSR environment may vary and is describe in detail below.

Data and project folders are stored based on the DUA covering the data. Currently, there are five major folders:

- emhsr_general
- emhsr_hcup
- emhsr_medicare
- emhsr_gediwise
- emhsr_ehr

Other folders may be created as new data is added to the environment.

Access is controlled using group permissions and access control lists on the folders and files. Access will not be granted to data folders until all of the requirements of the DUA have been met.

DUA subfolders:

emhsr_general - /sc/arion/projects/emhsr/emhsr_general/ - non-DUA controlled data and projects

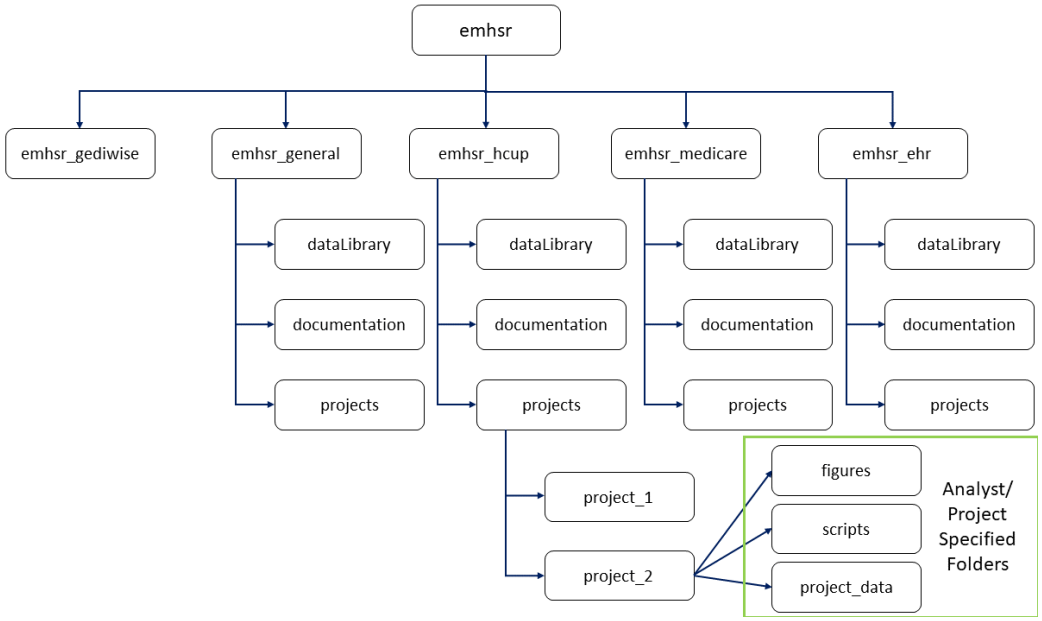
emhsr_hcup - /sc/arion/projects/emhsr/emhsr_hcup/ - raw data and projects covered by the HCUP DUA – users must sign the HCUP DUA and be listed on the project IRB

cmsdata - /sc/arion/cmsdata - raw and project data covered by the CMS DUAs held by Dr. Carr and supervised by Dr. Zebrowski

emhsr_gediwise - /sc/arion/projects/emhsr/emhsr_gediwise/ - any work affiliated with the GEDIWISE or Geri-ED research portfolio

emhsr_ehr - /sc/arion/projects/emhsr/emhs_ehr/ - projects utilizing EHR data from Mount Sinai or collaborating institutions

DUA subfolder Structure:



EMHSR Project Folders on Minerva

To maintain proper file permissions and access for backup, it is important that all projects workspaces are owned by the emhsr_admin user. To facilitate this, we have developed the below procedure for the creation of new project workspaces.

- When a new project is started on Minerva, email Alexis and Dave with:
- a brief description of the project
- the DUA the data falls under (CMS, HCUP, Mount Sinai EHR, etc)
- the desired directory name (short and descriptive, i.e. 'regards' (study acronym), 'mshs_wlst_ohca', etc.)
- Minerva usernames and permission (described below) for the research/analysis team
    - Read-only – user can view files in directory, but cannot edit or create new files/folders
    - Write – user can read/write/delete files in directory

User access and permissions can be updated and added as the project progresses.

Using LSF and Performing Analyses

Utilized LSF to schedule jobs…

Job submission parameters:

-J myfirstjob	# Job name
-P acc_hpcstaff	**# REQUIRED; To get allocation account, type "mybalance"**
-q premium	# queue; default queue is premium
-n 1	# number of compute cores (job slots) needed, 1 by default
-W 6:00	**# REQUIRED; walltime in HH:MM**
-R rusage[mem=4000]	# 4000 MB of memory request per "-n"; 3000 MB by default
-oo %J.stdout	# output log (%J : JobID)
-eo %J.stderr	# error log
-Is /bin/bash	# Specific to interactives - Initialize the execution environment

Batch Job Submission to LSF (General)

Sample command line and batch file text for simple job submission

gail01@li03c03: ~ $ *cat myfirst.lsf*

```
#!/bin/bash
#BSUB -J myfirstjob # Job name
#BSUB -P acc_hpcstaff # REQUIRED; To get allocation account, type "mybalance"
#BSUB -q premium # queue; default queue is premium
#BSUB -n 1 # number of compute cores (job slots) needed, 1 by default
#BSUB -W 6:00 # REQUIRED; walltime in HH:MM
#BSUB -R rusage[mem=4000] # 4000 MB of memory request per "-n"; 3000 MB by default
#BSUB -oo %J.stdout # output log (%J : JobID)
#BSUB -eo %J.stderr # error log
#BSUB -L /bin/bash # Initialize the execution environment

echo "Hello Chimera" # Command that you need to run
```

gail01@li03c03: ~ $ *bsub < myfirst.lsf*

Job <2937044> is submitted to queue <premium>.

Analytic Software - STATA

Running STATA in an INTERACTIVE session with GUI

- Login to Minerva – make sure you include the -X or -Y option
- Submit a job on the interactive queue
  - *bsub -P YOURALLOCATIONACCOUNT -q interactive -n 1 -W 01:00 -XF -Is /bin/bash*
    - Include project account after the -P flag
      - Replace *YOURALLOCATIONACCOUNT* with the Minerva project account, this name starts with acc_*
      - To see your project accounts run the *mybalance* command
    - Set wall time (how long the job is allowed to run) with the -W flag
      - There is no way to extend this time once you start the job! Plan accordingly.
    - Set number of nodes ("work slots") default is 1
    - The -XF flag is required to use the STATA GUI
- Load the Stata module
  - *module load stata*
  - If the module does not load, you may not have permission. Email the emhsr team to check
- Run xstata-mp

When you close the terminal window (or the connection is broken), the interative job will end. Even if it's in the middle of your analysis. Save frequently along the way and consider submitting a batch job if you are running a long complicated analysis.

Code block:

```
$   bsub -P YOURALLOCATIONACCOUNT -q interactive -n 1 -W 01:00 -R
rusage[mem=30000] -XF -Is /bin/bash
$   ml stata
$   xstata-mp
```

Typical output:

```
============================================================
[buckld05@li03c03 ~]$ bsub -P acc_emhsr_medicare -q interactive -n 1 -W 01:00 -XF -Is /bin/bash
Job <33324213> is submitted to queue <interactive>.
<<ssh X11 forwarding job>>
<<Waiting for dispatch ...>>
<<Starting on lc02a29>>
[buckld05@lc02a29 ~]$ module load stata
[buckld05@lc02a29 ~]$ xstata-mp
```

Installing SCC packages in STATA

In order to install and use custom packages in STATA, you must setup an http proxy in STATA.

```
set httpproxyhost 172.28.7.1
set httpproxyport 3128
set httpproxy on
```

Then you can install a package using the *ssc install* command. This can be done in an interactive session, or as part of a do file run within a batch job.

Submitting a STATA Batch job

Sample batch job file for STATA. This loads STATA and runs the analysis code contained within the do file specified.

```
#!/bin/bash
#BSUB -J myfirstjob              # Job name
#BSUB -P acc_hpcstaff            # REQUIRED; To get allocation account, type “mybalance”
#BSUB -q premium                 # queue; default queue is premium
#BSUB -n 1                       # number of compute cores (job slots) needed, 1 by default
#BSUB -W 6:00                    # REQUIRED; walltime in HH:MM
#BSUB -R rusage[mem=4000]        # 4000 MB of memory request per “-n”; 3000 MB by default
#BSUB -oo %J.stdout              # output log (%J : JobID)
#BSUB -eo %J.stderr              # error log
#BSUB -L /bin/bash               # Initialize the execution environment

module load stata16
stata-mp -b do <filename.do>
```

Troubleshooting Failed Jobs

If job launches, but then crashes:

- Run *bhist* to see how/why job shut down
- Check script output file (for Rstudio-on-the-fly and Jupyter Notebook)

If job shutdown because you exceeded the MEMLIMIT – request more memory when launching job

Analytic Software – R/RStudio

Running Rstudio

Option 1: On-the-fly Rstudio over Web in a Minerva job

- One simple command to get interactive web session in a HPC LSF job
- Available on login nodes only
- Containerized application for workflow reproducibility, packages installed in $HOME
    - Since this is a container env, you need to install/maintain your own R related packages.
- See usage with details:
    - `minerva-rstudio-web-r4.sh -h`
- Can specify non-default values for job submission variables. For example:
    - `minerva-rstudio-web-r4.sh -W 12:00 -P acc_PROJECT` – Will override the default wall time (6 hours, and set the project account to acc_PROJECT)

Typical Output:

```
[buckld05@li03c03 ~]$ minerva-rstudio-web-r4.sh -W 1:00 -n 1
[INFO] Image not specified, check if previously used
[INFO] Found previously used image /hpc/users/buckld05/minerva_jobs/rstudio_jobs/singularity-rstudio.simg. Using it.
[INFO] Project is not specified, or is acc_null, using 1st avail project.
[INFO] Project to use is acc_emhsr_medicare
[INFO] Parameters used are:
[INFO] -n       1
[INFO] -M       3000
[INFO] -W       1:00
[INFO] -P       acc_emhsr_medicare
[INFO] -J       rstudio
[INFO] -q       premium
[INFO] -R       null
[INFO] -i       /hpc/users/buckld05/minerva_jobs/rstudio_jobs/singularity-rstudio.simg
[INFO] Submitting rstudio job...
Job <33324635> is submitted to queue <premium>.
[INFO] See below for web access when job starts.
Job <33324635> : Not yet started.
[INFO] Job is pending
[INFO] Job is running, wait for link
<< output from stdout >>
Using local available port 8787
Using password in /hpc/users/buckld05/minerva_jobs/rstudio_jobs/.rstudio_onthefly_password
RStudio started in the singularity container with PID 144456.
Making sure it is alive
Checking 3, next check in 5 seconds.
   PID TTY          TIME CMD
144456 ?        00:00:00 singularity
Checking 2, next check in 5 seconds.
   PID TTY          TIME CMD
144456 ?        00:00:00 starter-suid
Checking 1, next check in 5 seconds.
   PID TTY          TIME CMD
144456 ?        00:00:00 starter-suid

SSH port forwarding to 10.95.46.103 with PID 144600.

Rstudio is started on compute node lc02g23, port 8787

Access the RStudio Web using your web browser:  http://10.95.46.103:54635


<< output from stderr >>
[buckld05@li03c03 ~]$
```

RStudio Package installation for RStudio-on-the-fly

More details in `minerva-rstudio-web-r4.sh -h`

Option 2: Run rstudio over XServer GUI

- Enable X11 forwarding and launch interactive job

```
bsub -P YOURALLOCATIONACCOUNT -q interactive -n 1 -W 01:00 -XF -Is
/bin/bash
ml rstudio
rstudio
```

Submitting a R Batch job

Sample batch job file for R. This loads R and runs the analysis code contained within the do file specified.

```
#!/bin/bash
#BSUB -J myfirstjob   # Job name
#BSUB -P acc_hpcstaff # REQUIRED; To get allocation account,
type "mybalance"
#BSUB -q premium      # queue; default queue is premium
#BSUB -n 1            # number of compute cores (job slots)
needed, 1 by default
#BSUB -W 6:00         # REQUIRED; walltime in HH:MM
#BSUB -R rusage[mem=4000]   # 4000 MB of memory request per "-n";
3000 MB by default
#BSUB -oo %J.stdout   # output log (%J : JobID)
#BSUB -eo %J.stderr   # error log
#BSUB -L /bin/bash    # Initialize the execution environment

module load R
R CMD BATCH [options] my_script.R [outfile]
```

Analytic Software – Python/Jupyter Notebook

Running Python

Option 1: On-the-fly Jupyter Notebook over Web in a Minerva job $ minerva-jupyter-web-r4.sh

- One simple command to get interactive web session in a HPC LSF job
- Available on login nodes only
- Containerized application for workflow reproducibility, packages installed in $HOME
    - Since this is a container env, you need to install/maintain your own python related packages.
- See usage with details:
    - $ *minerva-jupyter-web.sh -h*
- Can specify non-default values for job submission variables. For example:
    - $ *minerva-jupyter-web.sh -W 12:00 -P acc_PROJECT* – Will override the default wall time (6 hours, and set the project account to acc_PROJECT)

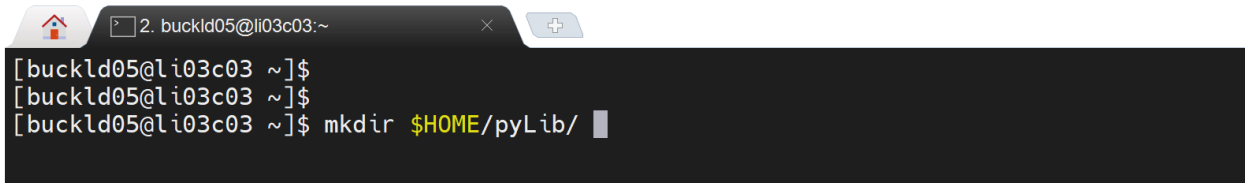
Submitting a Python Batch job

Sample batch job file for Python. This loads Python and runs the analysis code contained within the do file specified.

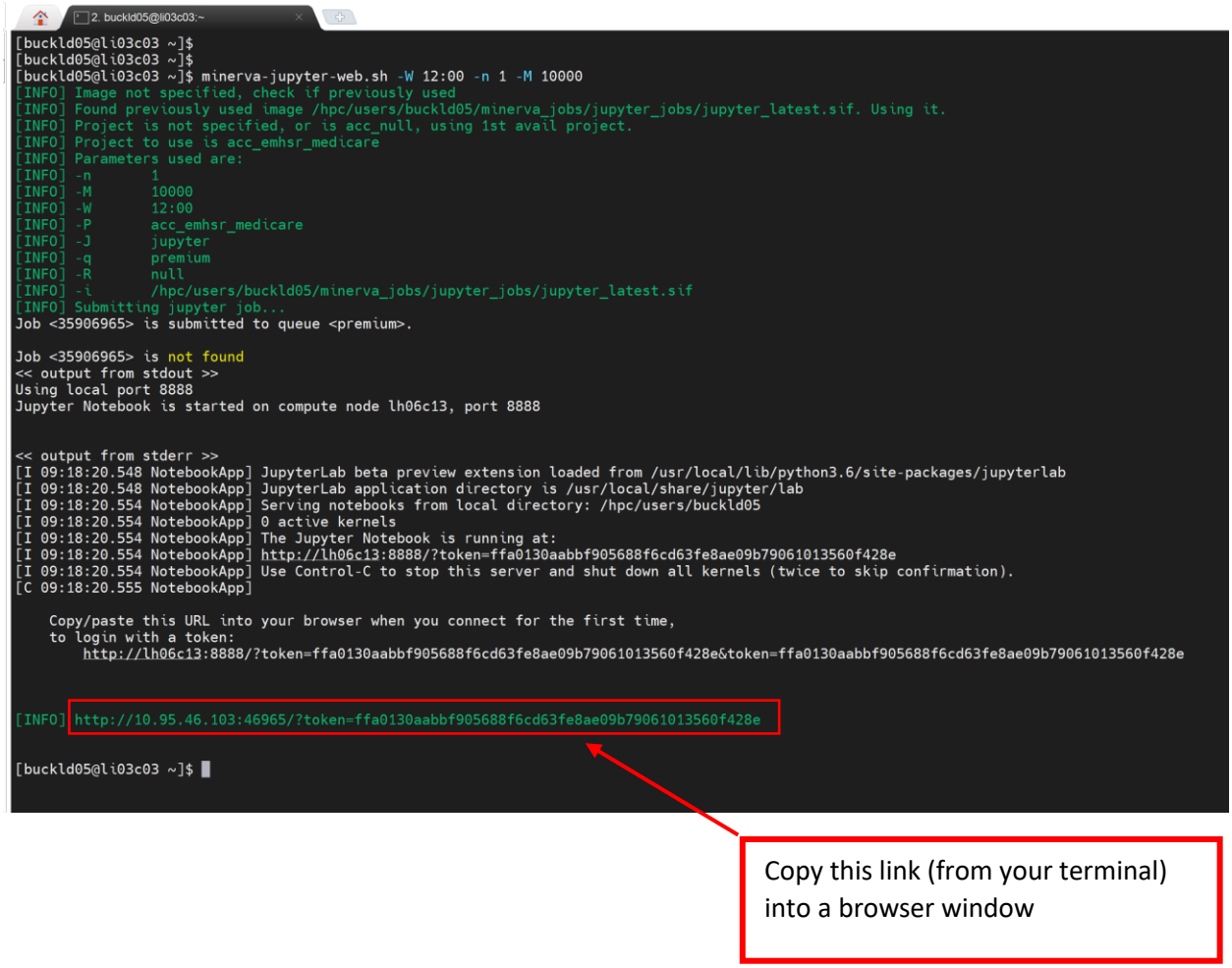
```
#!/bin/bash
#BSUB -J myfirstjob              # Job name
#BSUB -P acc_hpcstaff            # REQUIRED; To get allocation account, type “mybalance”
#BSUB -q premium                 # queue; default queue is premium
#BSUB -n 1                       # number of compute cores (job slots) needed, 1 by default
#BSUB -W 6:00                    # REQUIRED; walltime in HH:MM
#BSUB -R rusage[mem=4000]        # 4000 MB of memory request per “-n”; 3000 MB by default
#BSUB -oo %J.stdout              # output log (%J : JobID)
#BSUB -eo %J.stderr              # error log
#BSUB -L /bin/bash               # Initialize the execution environment

module load python/VERSION_NUMBER
python my_script.py [outfile]
```

Installing and using Python packages

1) Make a python library file in your home directory (I use pyLib as an example)

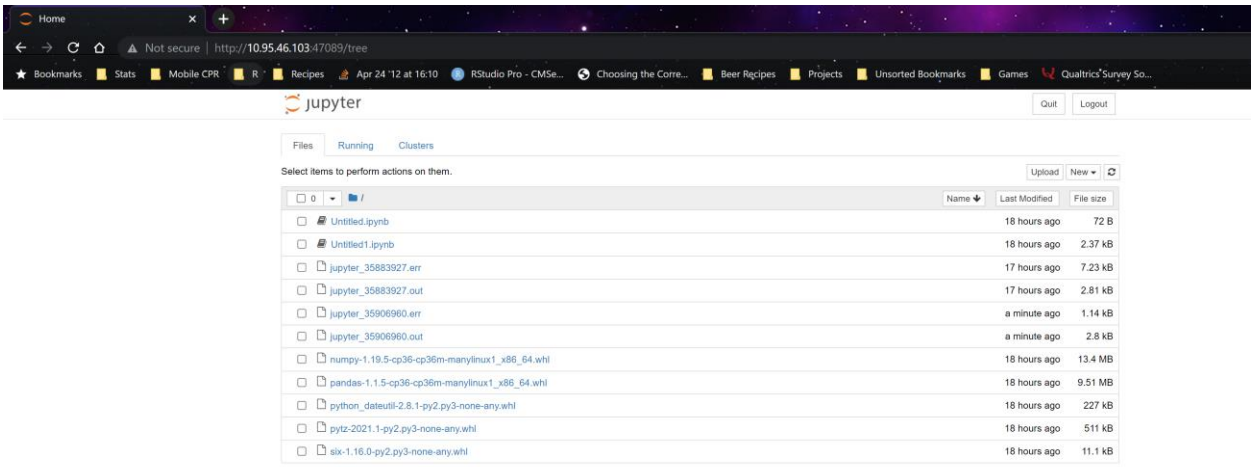


2) Launch jupyter notebook in a container on the HPC

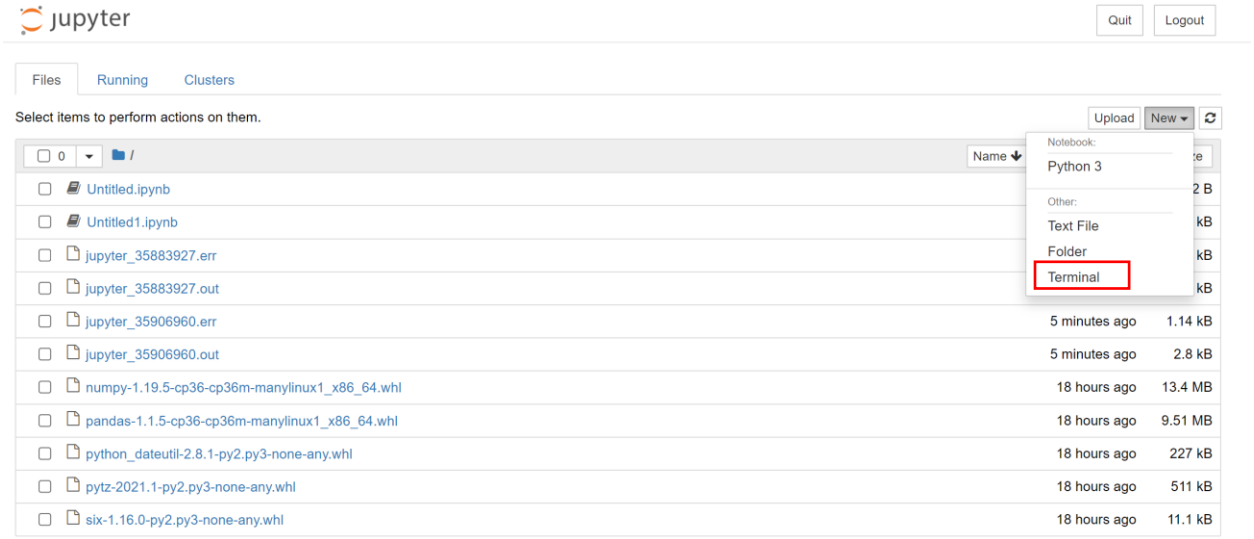


Copy this link (from your terminal) into a browser window

3) Connect to the notebook

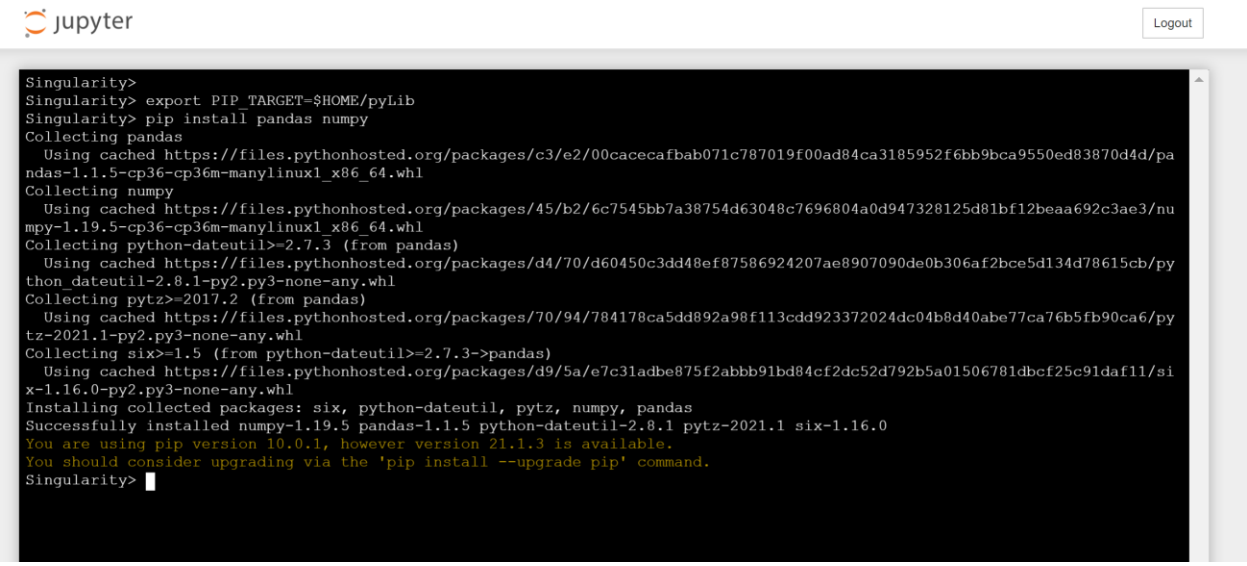


4) In Jupyer Notebook , open a terminal window:



5) In the Jupyter notebook terminal, run:

- export PIP_TARGET=$HOME/pyLib/
- pip install *packageName(s)*

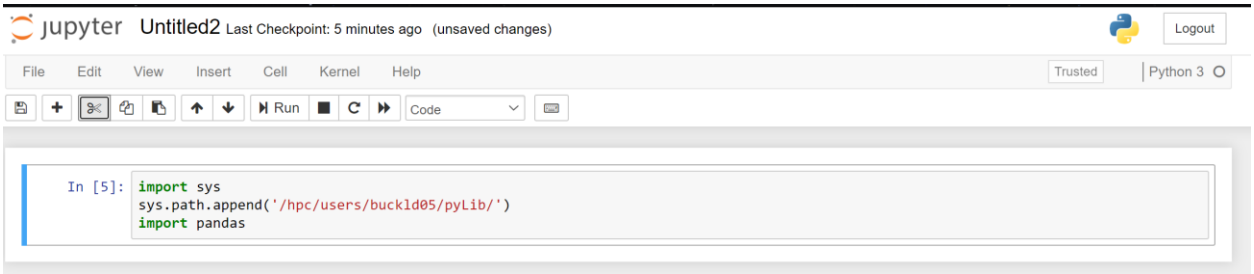


6) Close the terminal and open a Phython Jupyter Notebook

7) In python, run:

```
import sys
sys.path.append('/hpc/users/userName/pyLib/')
import pandas
```

Change *username* to be your username on Minerva. The $HOME environmental variable does not work in Jupyter notebook.



CMS Data Supplement

To comply with data safety requirements, all CMS research identifiable files (RIF) data and derived research files must be encrypted-at-rest. To accomplish this, the EMHSR analytics team and the Minerva HPC Team have setup a network file server (NFS) with whole disk encryption. This means that most users do not need to worry about encrypting their own working files before saving to disk.

The mount point for the CMS NFS is:

```
/sc/cmsdata
```

Login Node

As of 3/30/2022, the */sc/cmsdata* path is accessible on all login nodes. As always, the login node is for basic file management and job submission tasks. Do not run any analytic programs directly from the login node.

Once connected to a login node, you can navigate to the CMS data using the *cd* command:

```
cd /sc/cmsdata
```

Specifying compute nodes in a Batch Jobs

To utilize specific compute nodes when submitting a batch job to the LSF system, you must include a *-m* flag followed by the host, or range of hosts, you want to specify. This specification is in addition to the queue flag (*-q*) and the specified host(s) must be a part of the queue specified.

For example, if you are submitting a STATA batch job which uses this data your job script would look like this:

```
#!/bin/bash
#BSUB -J myfirstjob              # Job name
#BSUB -P acc_emhsr               # REQUIRED; To get allocation account, type “mybalance”
#BSUB -q premium                 # queue; default queue is premium
#BSUB -n 1                       # number of compute cores (job slots) needed, 1 by default
#BSUB -W 6:00                    # REQUIRED; walltime in HH:MM
#BSUB -R rusage[mem=4000]        # 4000 MB of memory request per “-n”; 3000 MB by default
#BSUB -oo %J.stdout              # output log (%J : JobID)
#BSUB -eo %J.stderr              # error log
#BSUB -L /bin/bash               # Initialize the execution environment

module load stata16
stata-mp -b do <filename.do>
```

Since more than 1 host is specified in the -m statement, the LSF will select the host(s) within the list what will allow the earliest dispatch of the job.

Inclusion in Interactive Jobs

The CMS NFS is now mounted on all of the hosts associated with the interactive queues. In order to initiate an interactive session on one of the nodes that can access the CMS NFS, include the *-m* argument along with the appropriate queue.

For example:

```
bsub -P acc_emhsr -q premium -n 1 -W 08:00  -Is /bin/bash
```

Will launch an interactive session on a CMS NSF host(s) in the premium queue for 8 hours. As before, if you need additional memory allocated, you will include a -R rusage[mem=XXXX] argument where XXXX represents the required memory size in MB.

Data Transfer - Minerva[1]

MSSM maintains high speed network connections with the commercial Internet and Internet2 through NYSERnet. MSSM currently maintains the following options for file transfer:

Globus Online:

When available, the **preferred** method for file transfer is Globus Online. The Globus Online software is required, which is free. It allows you to make parallel high speed transfers that can easily will a network connection. See instructions at Globus High Assurance HIPAA File Manager on Minerva.

SCP, SFTP, rsync

The standard transfer utilities, SCP, SFTP and rsync can be used to transfer files to and from MSSM systems. These utilities are usually already installed on Linux/Unix machines, and Mac's. There are also many command and graphical clients available. Due to familiarity and ease, these may be the best choice for transferring scripts and small files, however, these options can be slow in comparison, and may be ill suited for transferring large amounts of data, such as hundreds of TB's. More information on these utilities can be found on the transfer utilities page.

For windows, the best application for SCP is "PSCP". It is a command-line tool which replicates the Linux / Unix tools. It is very fast and efficient. You can acquire PSCP here.

A graphical alternative for Windows and Mac is CyberDuck. It is also quick, efficient, and full-featured.

Note: Ensure the Reuse password feature of CyberDuck is disabled. CyberDuck will try to reuse your one-use six-digit VIP token code repeatedly until you get locked out!

Physical Transport

We do support the copying of physical hard drives on the behalf of users. If you need files transferred this way, please provide us with drive to copy to / from and make a ticket with your request. Copies take several days. This service is done as a courtesy and is a best-effort service for bulk data transfer.

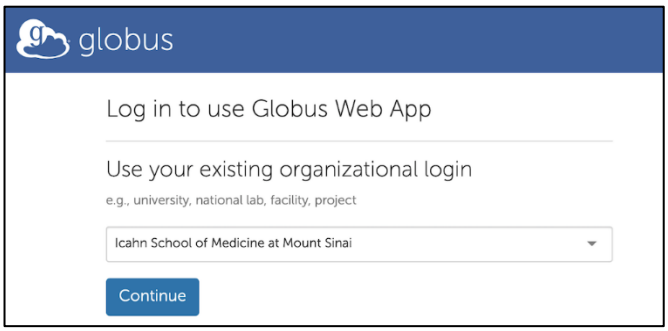
[1] Pulled from the Scientific computing website on 7/13/2021: https://labs.icahn.mssm.edu/minervalab/documentation/services/data-transfer/

Globus File Transfer

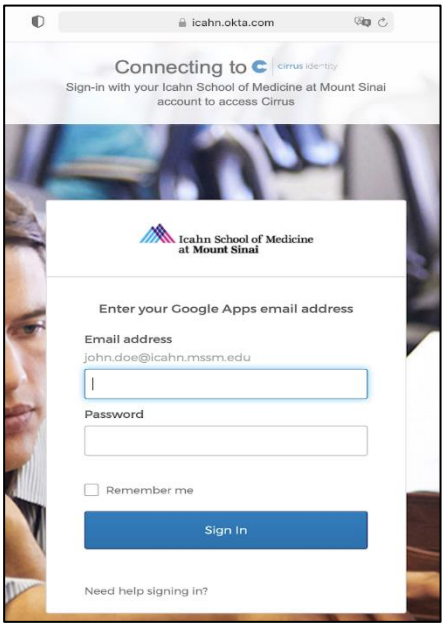
INDIVIDUAL USERS ARE RESPONSIBLE FOR ENSURING DATA TRANSFERRED OFF THE SERVERS COMPLY WITH THE DUA FOR THEIR DATA SOURCE. FOR MEDICARE, DATA MAY NOT BE TRANSFERRED OFF THE SERVERS IF IT CONTAINS IDENTIFIERS (BENE_ID, NAMES, DATES OF SERVICE) OR CELL COUNTS LESS THAN 11. IF YOU ARE UNCERTAIN ABOUT WHAT YOU ARE ALLOWED TO TAKE OFF THE SERVER, CHECK WITH ALEXIS AND DAVE.

How to login to Globus

To manage or share your Minerva files with collaborators, visit https://app.globus.org/ to login.



When prompted for authentication, please use your Mount Sinai school email (eg, first.last@mssm.edu) for access. If you are sure you have the correct username and password (no VIP), please contact ASCIT@mssm.edu for account activation with authentication services linked to https://icahn.okta.com/login/login.htm.



For users who are primarily Hospital or MSHS users, you may need to email ASCIT (ASCIT@mssm.edu) to ensure your user authentication service is set up. Before contacting ASCIT try the following:

1. Try to login with your first.last@mssm.edu and your school password (the one you use to log in to Minerva) NO VIP Token necessary.
2. If that does not work try username@mssm.edu and you school password.
3. If neither work, email ASCIT@mssm.edu using the template below and copy Igor Bodner (igor.bodner@mssm.edu), as well as Alexis and Dave so we can help troubleshoot.

I currently have access to the Minerva environment, but I am unable to log-in and authenticate my Globus account via https://app.globus.org/.

My MSSM login (used to access Minerva) is **userName**. Can you please enable my MSSM account for globus?

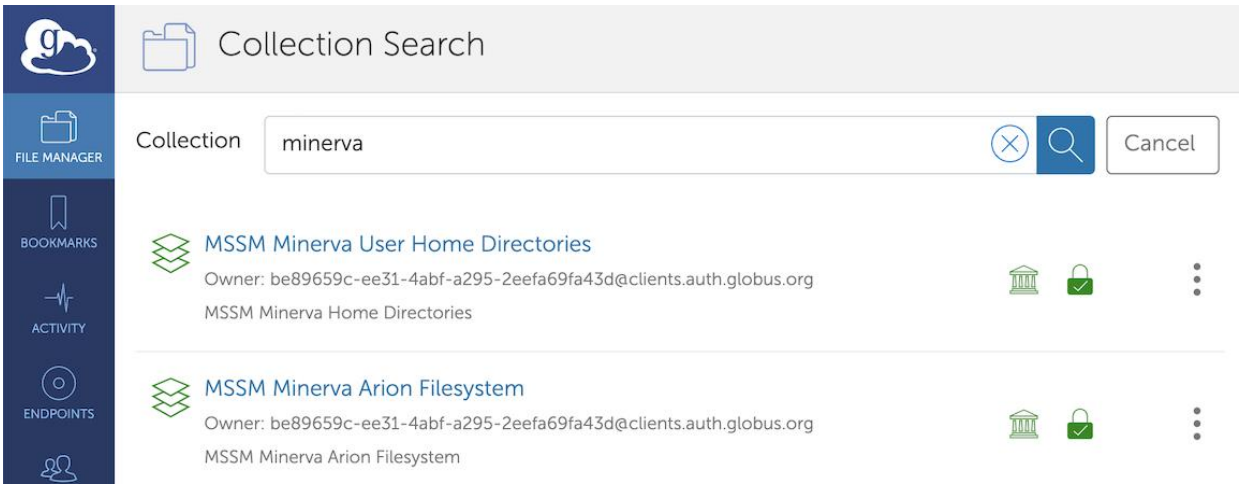
Please let me know if there is any additional information you need for this request.

Thank you,

Your Name Here

Minerva collections available

After login, in the File Manager tab, search Minerva in the collections. Please use the following two collections to access your files under /sc/arion and your files under home /hpc/users. Watch the owner id be89659c-xxx.



How to Share files with Globus?

If you are uploading a small amount of data from the local computer, you can use the "Upload" option in the globus file manager (app.globus.org). This only works if you are logged into your account and can navigate to the destination directories.
If you are transferring large quantities of data to Minerva, you will want to set up a Globus Personal Endpoint on your laptop or desktop. The personal endpoint will manage the transfer process for you, including pausing and restart the transfer if your connection is dropped.

If you are transferring PHI/PII, you will need to setup your personal endpoint with "High Assurance" and email the Minerva HPC team (hpchelp@hpc.mssm.edu) to be added to the Managed Endpoints list. If you think this is necessary, check with Alexis and Dave first.

Other Useful commands

$ mybalance

Displays the Project names you have access to. A project name from this list needs to be included with all job submissions after the -P switch

$ quota

Displays the storage space used by your user and what portion of the allotted space you have used

$ screen

When a connection to a remote server is lost, a signal (HUP) is sent to all running processes to shutdown. The screen command allows command line processes to continue to run after HUP and lets the user reconnect to the process after reconnection. Screen also allows user to have multiple command lines open at the same time. Screen does NOT keep X-server applications (like xstata or sas) open. The base program will continue to run, but the user may not be able to connect to the running graphical user interface (GUI) for the program.