Introduction to Minerva

Minerva Scientific Computing Environment

https://labs.icahn.mssm.edu/minervalab

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Mount
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Outlines

- Compute and storage resources
- Account and logging in
- User software environment
- Other services on file transfer, data archive, and web server

Minerva cluster @ Mount Sinai

Chimera Partition:

- 3x **login nodes** - Intel 8168 24C, 2.7GHz - **384 GB** memory
- Compute nodes -
  - 275 **regular memory nodes** - Intel 8168 24C, 2.7GHz - 48 cores per node - **192 GB**/node)
  - 37 **high memory nodes** - Intel 8168/8268, 2.7/2.9GHz - **1.5 TB** mem
  - **GPU nodes:**
    - 12 -Intel 6142, 2.6GHz - 384 GB memory - 4x V100-**16 GB** GPU
    - 8 - Intel 8268, 2.9 GHz - 384 GB memory - 4x A100- **40 GB** GPU
      - 1.8 TB SSD per node
    - 2 - Intel 8358,2.6GHz - 2 TB memory - 4x A100- **80 GB** GPU
      - 7 TB SSD per node, NVlink

NIH FUNDED NODES

BODE2 Partition:

- $2M S10 BODE2 awarded by NIH (Kovatch PI)
- 78 compute nodes - Intel 8268, 2.9 GHz -48 cores per node - **192 GB**/node

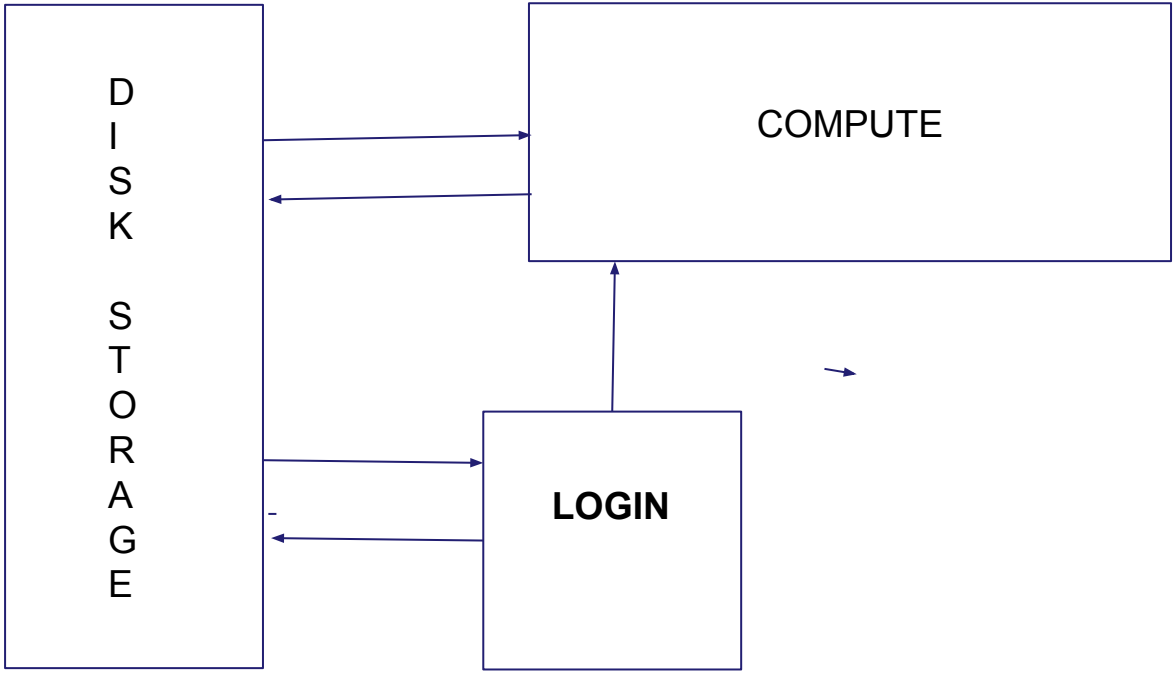
CATS Partition:

- $2M CATS awarded by NIH (Kovatch PI)
- 55 compute nodes - Intel 8358, 2.6 GHz- 64 cores per node -**1.5 TB** / node

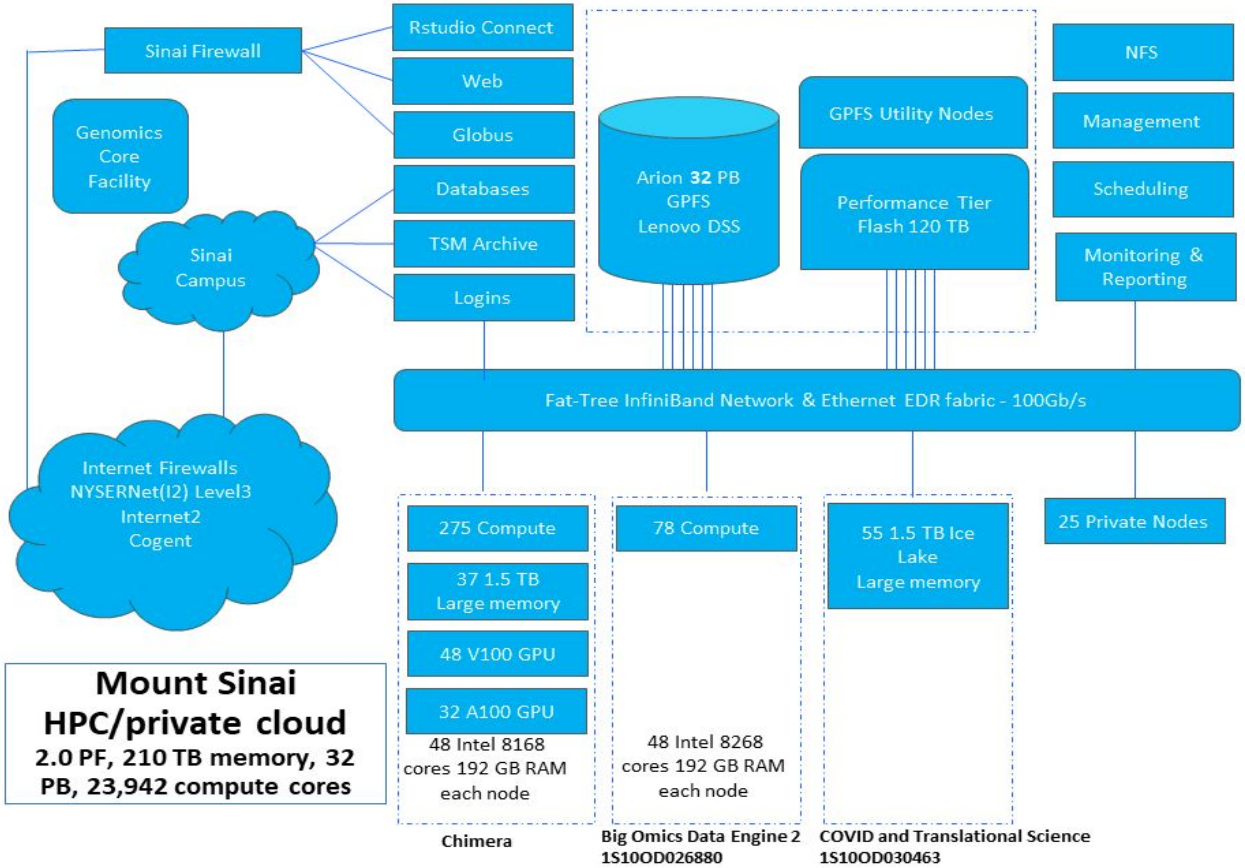
Storage: 32PB of high-speed online storage as an IBM General Parallel File System (**GPFS**)

- **Path /sc/arion** : Use the system path environment variable in scripts **$GPFS**

Minerva Cluster from 30,000 ft.



Minerva Cluster@ Mount Sinai



HIPAA

- Minerva is HIPAA compliant as of October 1st, 2020, i.e., Protected Health Information (PHI) data is allowed to be stored and processed on Minerva.

- All users have to read the HIPAA policy and complete Minerva HIPAA Agreement Form **annually** (every Jan.) at https://labs.icahn.mssm.edu/minervalab/hipaa/

- Users who have not signed the agreement will have their accounts locked until the agreement is signed.

General Minerva Information

- The Minerva website is:

  https://labs.icahn.mssm.edu/minervalab/

  or

  https:www.hpc.mssm.edu

  - Contains the documentation for the features and access to the forms
- Access to Minerva requires a Minerva userid
  - Not automatic. You need to apply for one.
  - Username will be the same as your Mount Sinai Login id.
  - Link to form off of Scientific Computing home page or https://labs.icahn.mssm.edu/minervalab/request-an-account/

Logging in

Minerva is a Linux machine with Centos 7.6

- Linux is command line based, not GUI (But we have a gui wrapper: OnDemand)
- Logging in requires campus network, **SSH client** installed on your machine, **username, memorized password,** and **one-time code** obtained from a Symantec VIP token

Detailed procedures:

- Campus network (School VPN needed if off-campus)
- Apply for an account at https://acctreq.hpc.mssm.edu/
  - Apply account for external users following here
- Complete HIPAA form at https://labs.icahn.mssm.edu/minervalab/hipaa/ to activate your account
- Register your token at the Self Service Portal **school site** (https://register4vip.**mssm**.edu/vipssp/)
- SSH client: terminal (Mac), MobaXterm/Putty (Windows)
- Logging info at https://labs.icahn.mssm.edu/minervalab/logging-in/

*Note: Minerva is school resource, so use your **school password and school portal** for register*

Migration from Symantec VIP to Azure MFA

- DTP is in the process of migrating to Azure MFA
- Planned cutover from Symantec to Azure for Minerva is late 2024 (when VPN is fully with Azure MFA)
  - All users of Minerva need to register for MFA in preparation https://itsecurity.mssm.edu/mobile-device-security/ms-authenticator/
- In the meantime, for **new users**, to use VIP token to access Minerva
  - Need to first get access to VPN or school email; then register VIP token
  - If no VPN or school email account, then you need to request a role via Sailpoint "**Azure MFA and Symantec VIP Token Registration"**

Logging in - Linux / Mac

Connect to Minerva via ssh

- Open a terminal window on your workstation
- ssh *your_userID*@minerva.hpc.mssm.edu
- To display graphics remotely on your screen, pass the “-X” or “-Y” flag:
  - ssh -X *your_userID*@minerva.hpc.mssm.edu
  - Mac: Install XQuartz on your mac first
  - Test by running the command: xclock
    - Should see a clock
- Landed on one of the login nodes, and at your home directory
  - Never run jobs on login nodes
  - For file management, coding, compilation, check/manage jobs etc., purposes only
  - Basic linux command**: cd, ls and more**

```
imac:~ gail01$ ssh -X gail01@minerva.hpc.mssm.edu
Please input your password and two factor token:
Password:
Last login: Mon Sep 13 16:24:06 2021 from 10.254.167.11
================================================================
Run "Minerva_help" for useful Minerva commands and websites

   === Upcoming Minerva Training Sessions ===
Session 1: 15 Sep 2021, 11:00AM-12:00PM – Introduction to Minerva
Session 2: 22 Sep 2021, 11:00AM-12:00PM – LSF Job Scheduler
Session 3: 29 Sep 2021, 11:00AM-12:00PM – Globus: Data Transfer
Zoom link for all sessions:
https://mssm.zoom.us/j/5420563013


   === Send ticket to hpchelp@hpc.mssm.edu ===
WE DO NOT BACKUP USER FILES
        PLEASE ARCHIVE/BACKUP YOUR IMPORTANT FILES
   === Send ticket to hpchelp@hpc.mssm.edu ===
================================================
gail01@li03c04: ~ $ pwd
/hpc/users/gail01
gail01@li03c04: ~ $ xclock
```

```
gail01@li03c02: ~ $ minerva_help

Our Minerva HPC website:          https://labs.icahn.mssm.edu/minervalab/
Our lastest Slides:
Basic Minerva Enviorment https://labs.icahn.mssm.edu/minervalab/wp-content/uploads/sites/342/2020/10/Minerva_Intro_-2020-09-16.pdf
Advanced LSF job scheduler https://labs.icahn.mssm.edu/minervalab/wp-content/uploads/sites/342/2020/09/Minerva_LSF_2020-09-23.pdf

Publish R/shiny to Rstudio Connect server: https://labs.icahn.mssm.edu/minervalab/rstudio-connect-server/
Data transfer:                    https://labs.icahn.mssm.edu/minervalab/data-transfer/
Web service:                      https://labs.icahn.mssm.edu/minervalab/web-services/
TSM data archive:                 https://labs.icahn.mssm.edu/minervalab/archiving-data/

Useful Commands

Check limits on login nodes:      ulimit -a
Modules:
Show all available modules:       ml avail
Load module:                      ml <package name>
List loaded modules:              ml list
Unload a module:                  ml -<package name>
Remove all loaded modules:        ml purge

Run rstudio over GUI:             ml rstudio; rstudio
Run rstudio over web:             minerva-rstudio-web.sh (with details at https://labs.icahn.mssm.edu/minervalab/rstudio-web/)

Check available accounts for computes: mybalance
Submit job to LSF job scheduler: bsub < my_lsf_script.sh
see a list of your jobs:          bjobs
check currentjob in long format: bjobs -l jobID
List all compute nodes:           bhosts
List high memory nodes:           bhosts himem
List gpu nodes:                   bhosts gpu
List interactive nodes:           bhosts interactive
List all available LSF queues:    bqueues
```

Logging in - Windows

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

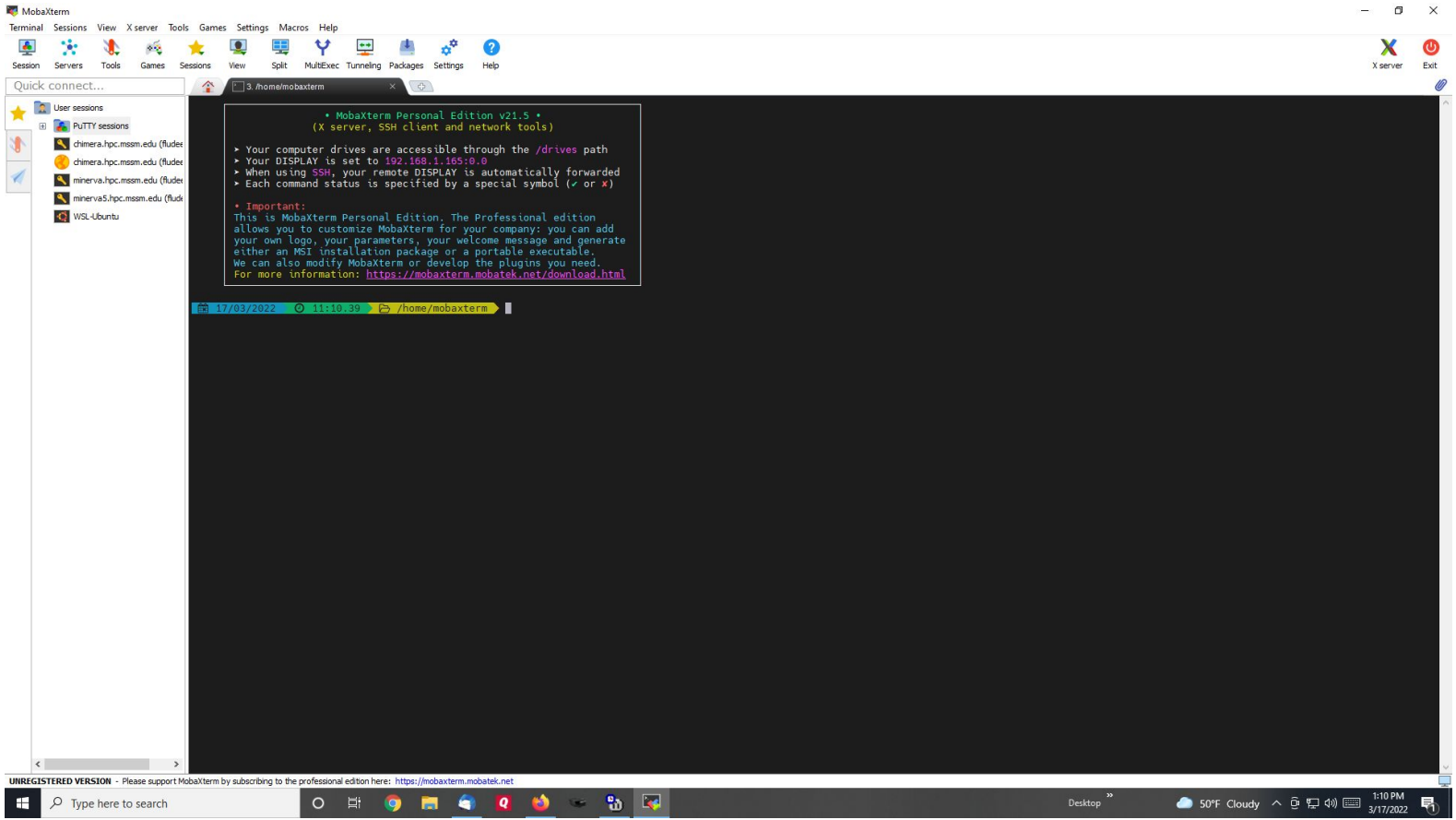
OR

- **Install PuTTY from www.putty.org**
  - Google it. It will be the first hit https://www.youtube.com/watch?v=ma6Ln30iP08
  - 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
    - Google; Download; Follow bouncing ball
  - Test by logging into Minerva and run the command: xclock
    - Should see a clock

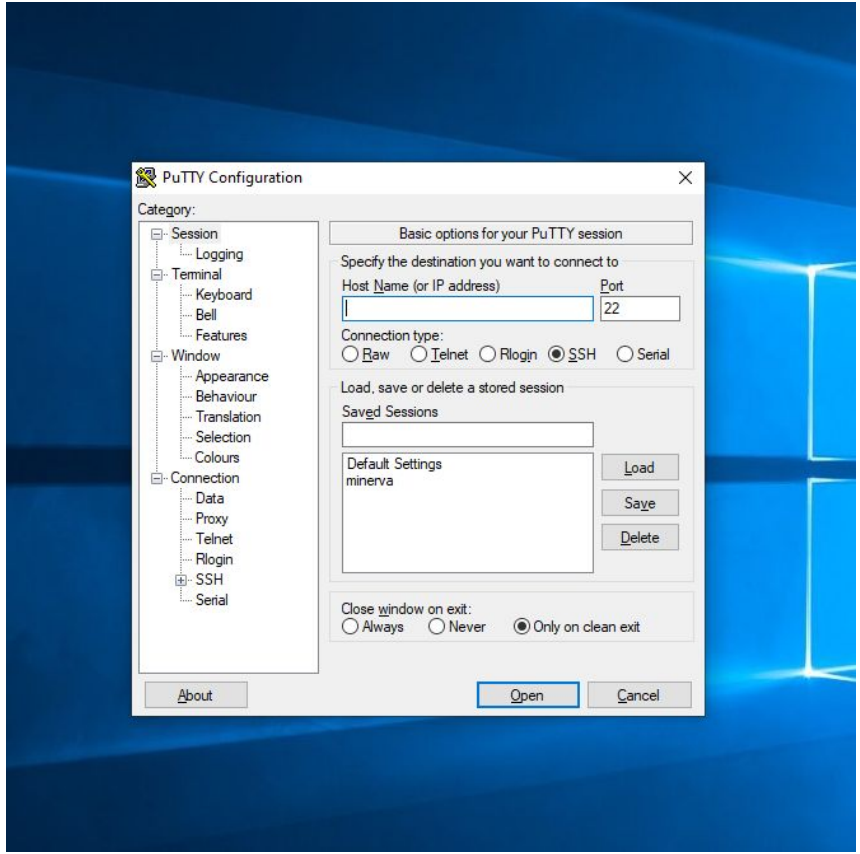
OR

- **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 dualboot setup

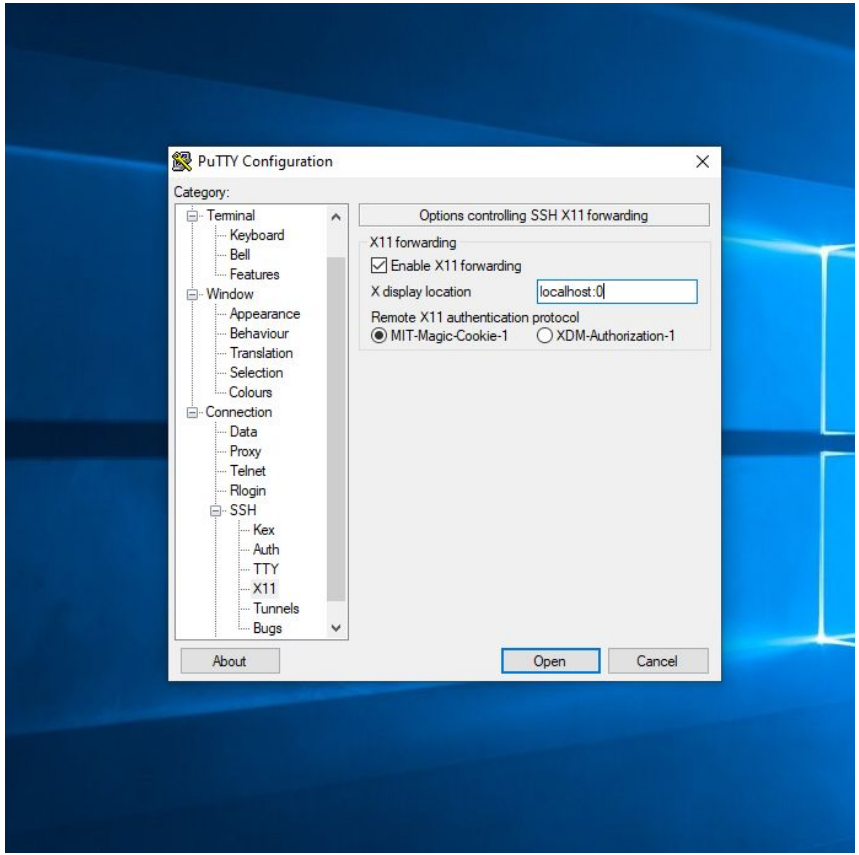
MobaXterm


MobaXterm
Terminal Sessions View X server Tools Games Settings Macros Help
Session Servers Tools Games Sessions View Split MultiExec Tunneling Packages Settings Help
X server Exit
Quick connect...
User sessions
PuTTY sessions
chimera.hpc.mssm.edu (fluder
chimera.hpc.mssm.edu (fluder
minerva.hpc.mssm.edu (fluder
minerva5.hpc.mssm.edu (fluder
WSL-Ubuntu
3. /home/mobaxterm
• MobaXterm Personal Edition v21.5 •
(X server, SSH client and network tools)
➤ Your computer drives are accessible through the /drives path
➤ Your DISPLAY is set to 192.168.1.165:0.0
➤ When using SSH, your remote DISPLAY is automatically forwarded
➤ Each command status is specified by a special symbol (✔ or ✘)
• Important:
This is MobaXterm Personal Edition. The Professional edition
allows you to customize MobaXterm for your company: you can add
your own logo, your parameters, your welcome message and generate
either an MSI installation package or a portable executable.
We can also modify MobaXterm or develop the plugins you need.
For more information: https://mobaxterm.mobatek.net/download.html
17/03/2022 11:10.39 /home/mobaxterm
UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: https://mobaxterm.mobatek.net
Type here to search
Desktop
50°F Cloudy
1:10 PM
3/17/2022

Putty- Initial Screen



Putty= X11 screen



Logging in - login nodes

3 login nodes: minerva[12-14], which points to the login node **li03c[02-04]**

- only available within campus-network

Users	Login method	Login servers	Password Components
Sinai users	userID	**@minerva.hpc.mssm.edu** **or specific nodes:** **@minerva12.hpc.mssm.edu** **@minerva13.hpc.mssm.edu** **@minerva14.hpc.mssm.edu**	Sinai Password followed by 6 Digit Symantec VIP token code
External users			

Note: Load balancer **Round-robin** is configured for **minerva.hpc.mssm.edu.** It will distribute client connections to the nearest across a group of login nodes.

Logging in - Config file

- **~/.ssh/config at your local workstation**
- **%USERPROFILE%\.ssh\config on Windows**
  - Set ControlMaster to reuse ssh connection for all hosts
  - Enable X11 forwarding
  - Set alias for hostname, so just type **ssh minerva** for login

```
$ cat ~/.ssh/config
Host *
        ControlMaster auto
        ControlPath /tmp/ssh_mux_%h_%p_%r
        ControlPersist 24h
        PreferredAuthentications        keyboard-interactive
        ServerAliveInterval 240
        ServerAliveCountMax 2
        ForwardX11 yes
        ForwardX11Timeout   12h

Host minerva
        Hostname minerva.hpc.mssm.edu
        User gail01
```

Minerva Storage

- Storage is in folders and subfolders. In linux, subfolders are separated by “/”
- 4-ish 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

User Software Environment: Lmod

> 1000 modules, and different versions are supported on Minerva

Lmod Software Environment Module system implemented:

- Search for module: **$module avail** or **$ module spider**
  Check all available R versions *$ ml spider R*

  …….R/3.3.1, R/3.4.0-beta, R/3.4.0, R/3.4.1, R/3.4.3_p, R/3.4.3, R/3.5.0, R/3.5.1_p, R/3.5.1, R/3.5.2, R/3.5.3
- To check the detailed PATH setting in module files: **$ml show R**
- Load module: **$ml python or $module load python** or **$ml python/2.7.16** (for a specific version)
- Unload module **$ml -gcc or $module unload gcc**
- List loaded modules: **$ml or $module list**
- Purge ALL loaded modules **$ ml purge**
- Autocompletion with tab
- More at Lmod user guide

```
gail01@li03c03: ~ $ ml python
gail01@li03c03: ~ $ ml

Currently Loaded Modules:
  1) gcc/8.3.0   2) python/3.7.3



gail01@li03c03: ~ $ ml python/2.7.16

The following have been reloaded with a version change:
  1) python/3.7.3 => python/2.7.16

gail01@li03c03: ~ $ ml -gcc
```

User Software Environment - Major packages

OS: **Centos 7.6** with **glibc-2.17(GNU C library) available**

GCC: system default /usr/bin/gcc is gcc 4.8.5

$ module load gcc (default is 8.3.0) or *$ ml gcc*

$ ml python Python: default version 3.7.3 (it will load python and all available python packages)

Note: python2 or python3 *$ml python/2.7.16*

$ ml R R: default version 4.2.0 it will load R and all available R packages)

$ml CPAN Collection of system Perl software: default system version 5.16.3

$ml anaconda3 Anaconda3: default version 2018-12

$ml java java: default version 1.8.0_211

SAS access: *$ml sas*

- The cost for the license is **$150.00** per activation, and request form at here

Matlab access: *$ml matlab*

  - The cost for the license is **$100.00** per activation, and request form at here.

User Software Environment - Anaconda Distribution

- Anaconda3/Anaconda2: Support minimal conda environments (such as tensorflow, pytorch, qiime) e.g., tensorflow (both in CPU and GPU)
- **To avoid incompatibilities with other python, clear your environment with module purge before loading Anaconda**

  $ml purge

  $ml anaconda3/2020.11

  $conda env list ***# get a list of the env available (Or*** *$conda info --envs)*

  source activate tfGPU2.4.1
- User should install their own envs locally, (see more guide here)
  - ➔ Use option -p PATH, --prefix PATH Full path to environment location (i.e. prefix).

    $conda create python=3.x -p /sc/arion/work/gail01/conda/envs/myenv

    $conda env create -p myenv -f environment.yml
  - ➔ Set envs_dirs and pkgs_dirs in .condarc file, specify directories in which environments and packages are located

    $conda create -n myenv python=3.x
- Set conda base auto-activation false

  conda config --set auto_activate_base false

  More at Conda config guide

```
$ cat ~/.condarc file
envs_dirs:
- /sc/arion/work/gail01/conda/envs
pkgs_dirs:
- /sc/arion/work/gail01/conda/pkgs
conda config --set auto_activate_base false
```

User Software - Singularity Container Platform

Singularity tool is supported, instead of docker (Security concern)

- Docker gives superuser privilege, thus is better at applications on VM or cloud infrastructure
- It allows you to create and run containers that package up pieces of software in a way that is portable and reproducible. Your container is a single file and can be ran on different systems

To load singularity module: *$ module load singularity/3.11.0*

To pull a singularity image: *$ singularity pull --name hello.simg shub://vsoch/hello-world*

To create a container within a writable directory (called a sandbox):

$singularity build --sandbox lolcow/ shub://GodloveD/lolcow (create container within a writable directory)

To pull a docker image: *$singularity pull **docker://**ubuntu:latest*

To shell into a singularity image: *$ singularity shell hello.simg*

To run a singularity image: *$ singularity run hello.simg*

To get a shell with a specified dir mounted in the image

$ singularity run -B /user/specified/dir hello.simg

Note: /tmp, user home directory, and /sc/arion/is automatically mounted into the singularity image.

User Software - Singularity Container

To build a new image from recipe file/definition file:

Use Singularity **Remote Builder** or your local workstation

- Singularity build is not fully supported due to the sudo privileges for users
- Using the Remote Builder, you can easily and securely create containers for your applications without special privileges or set up in your local environment
- Write your recipe file/definition file https://sylabs.io/guides/3.6/user-guide/definition_files.html
- Convert docker recipe files to singularity recipe files:

  $ml python

  $spython recipe Dockerfile Singularity

For more information about Singularity on Minerva, please check our training slide here

User Software - How to Run Jupyter Notebook

One simple command to get interactive **web** sessions in a HPC LSF job (Available on login nodes only) with details here

Option1: $minerva-jupyter-module-web.sh (--help to get help message/usage)

[INFO] This script is to submit a Python Jupyter Notebook web instance inside an
[INFO] LSF job on ***one single host*** for users.
[INFO] By default, this script uses Jupyter from **python/3.7.3**
[INFO] You can load other ***python version and other modules needed*** for your Jupter Notebook by -mm option

You can load Minerva modules needed for your Jupyter Notebook

Option 2: $minerva-jupyter-web.sh (--help to get help message/usage)

[INFO] This script is to submit a ***Singularity containerized*** Jupyter Notebook web instance inside an
[INFO] LSF job on ***one single host*** for users.
[INFO] By default, this script uses this **Singularity image** (shub://ISU-HPC/jupyter)

For users who want an isolated/clean env working with container image. You need to install/maintain your own python related package. No module system setup

User Software - How to Run Jupyter Notebook

Option 1 (con't): Access Jupyter notebook running on Minerva compute node via port forwarding

1) You can use one simple command wrapper mentioned above:$minerva-jupyter-module-web.sh

OR

2) Issue commands step by step with more control by yourself:

start an interactive session for example

$bsub -P acc_xxx -q interactive -n 2 -R "span[hosts=1]" -R rusage[mem=4000] -W 3:00 -Is /bin/bash

#Then on the allocated nodes lc01c30, start Jupyter Notebook

lc01c30 $ml python

lc01c30$jupyter notebook --no-browser --port=8889

#On your local workstation, forward port XXXX(8889) to YYYY(8888) and listen to it

$ssh -t -t -L localhost:8888:localhost:8889 gail01@minerva.hpc.mssm.edu ssh -X lc01c30 -L localhost:8889:localhost:8889

#Open firefox on local: http://localhost:8888

* note: you can change the portal number 8888/8889 to others

User Software - How to Run Jupyter Notebook

Option 2 (con't): On-the-fly Jupyter Notebook in a Minerva job $minerva-jupyter-web.sh

- Containerized application for workflow reproducibility, packages installed in $HOME/.local
- See usage: `minerva-jupyter-web.sh -h`
- No module system setup.

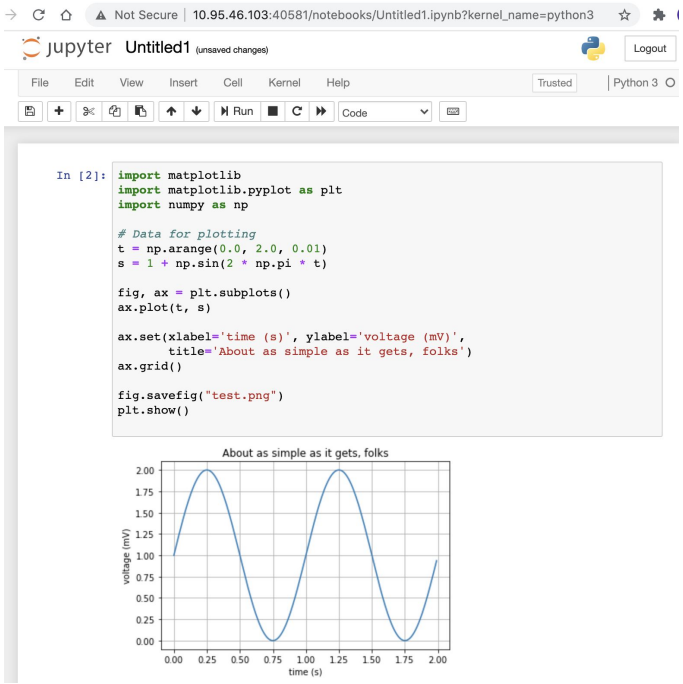
To install your own python packages:

- Open the terminal in web the jupyter web, type

```
pip install packages
--user
```

This will be in your home directory $HOME/.local.

restart the jupyter notebook



User Software - How to Run Jupyter Notebook

Summary

	minerva-jupyter-module-web.sh	minerva-jupyter-web.sh
Access modules on Minerva	Yes	No
Using singularity image	No	Yes
Support GPU node	Yes	Yes
Python versions	By default, python/3.7.3; You can load other *python version and other modules needed* for your Jupter Notebook by -mm option	This script uses the python within this Singularity image (shub://ISU-HPC/jupyter)
Others	For users who want to access Minerva modules.	For users who want an isolated/clean env working with a container image. You need to install/maintain your own python related package. No module system setup

User Software - Rstudio

Option 1: On-the-fly Rstudio over Web in a Minerva job $minerva-rstudio-web-r4.sh

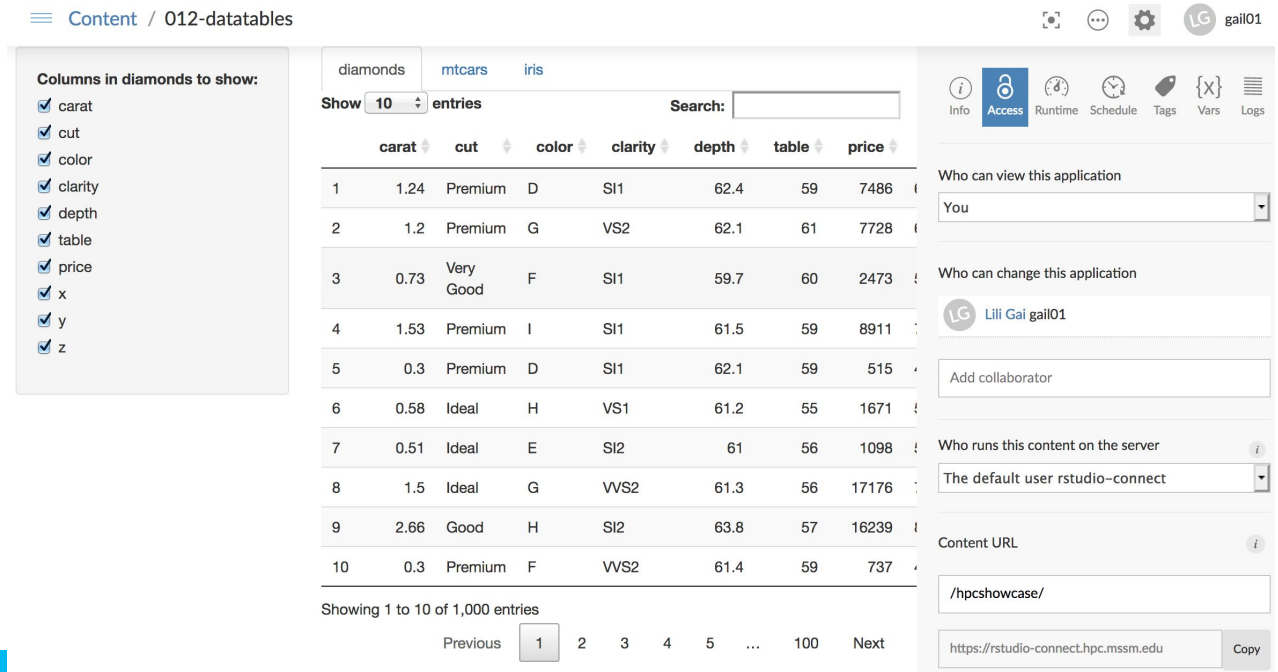
- One simple command to get interactive **web** sessions in a HPC LSF job
- Available on login nodes only
- Containerized application for workflow reproducibility, packages installed in $HOME
  - Since this is a container env, you need to install/maintain your own R related package. No module system setup.
- See usage with details:
  - `minerva-rstudio-web-r4.sh -h`

Option 2: Run rstudio over GUI (graphical user interface)

- Enable X11 forwarding (see P.7 & P.9)
- ml rstudio; rstudio

Posit Connect (formerly Rstudio Connect) server https://rstudio-connect.hpc.mssm.edu

- You can publish Shiny, R Markdown for collaborators or others
- If interested in publishing on Rstudio-connect, please check instruction at https://labs.icahn.mssm.edu/minervalab/documentation/r/#rstudioconnect



User Software Environment - some config

- You can load modules in your **.bashrc** script to load them on startup

  or check out User Collections:

https://lmod.readthedocs.io/en/latest/010_user.html#user-collections-label

- You can create your own modules and modify MODULEPATH so they can be found by

  module use /hpc/users/fludee01/mymodules

  or

  export MODULEPATH=/hpc/users/fludee01/mymodules:$MODULEPATH
- You can set PATH or PYTHONPATH by

  export PATH=/hpc/users/gail01/.local/bin:$PATH

  export PYTHONPATH=/hpc/users/gail01/.local/lib/python3.7/site-packages:$PYTHONPATH

File Transfer - Globus (Preferred)

- Globus is developed/maintained at the University of Chicago and used extensively at HPC centers
- Globus makes it easy to move/sync/share **large amounts of data**.
- Globus will **retry failures, recover from faults automatically when possible, and report the status of your data transfer**. Globus website

Globus on Minerva under HIPAA+BAA subscription

- *Be able to share data with their identity/email address. No Minerva account needed*
- *Can upgrade your Globus account to Plus, enabling file transfer between two personal Globus endpoints and data share from a Globus Connect Personal endpoint*

Data transfer with Globus on Minerva (see instructions here)

- *Login to Globus with Mount Sinai school email (eg, first.last@mssm.edu)*
- *Minerva collections: MSSM Minerva User Home Directories and MSSM Minerva Arion FileSystem*
- ***Use HTTPS for download/upload:** Now you can move data within your browser, without installing Globus Connect Personal; you'll see options for upload and download in the Globus web app.*
- *Users handling HIPAA/sensitive data on machines running Globus Connect Personal, please check High Assurance in the preference*

File Transfer - Con't

- **SCP, SFTP**
  - Good for relatively small files, not hundreds of TB's. Not recommended.
  - *Some scp apps for Windows/Mac use cached password. This feature must be turned off.*
  - *ftp is not supported on Minerva due to security risk*
  - *Note when you use VPN, data transfer between Minerva and your local computer may be pretty slow because the bandwidth is limited by school IT*

- **On Minerva**
  - After login to Minerva, ssh *li03c01* for data transfer, no time limit
  - minerva12/13/14 (33h) or interactive nodes (12h).
  - Please use a screen session so that you can return to your work after the drop of the connection.

Archiving Data: IBM Tivoli Storage Management (TSM)

- Keep for 6 years with two copies
- Can be accessed via either a GUI or the command line

```
$ module load java
$ dsmj -se=userid
```

or

```
$ dsmc -se= userid
```

- Large transfers can take a while. Use a ***screen*** session and disconnect to prevent time-outs
- Full more details here
- **Collaboration account:**
  - If your group needs a collaboration account for group related tasks like archiving a project directory or managing group website, please check https://labs.icahn.mssm.edu/minervalab/minerva-quick-start/collaboration-account

Web server

- Your website at **https://userid.u.hpc.mssm.edu**
- The document root for a user's site is within home folder in a folder called ~/www
- **NO PHI may be shared via the webserver.**

Step 1: Create ~/www. `$ mkdir ~/www`

Step 2: Place content (eg. index.html) put files or create symlink (from arion) in the www folder

```
$ cat > ~/www/index.html <<EOF
Hello World from my website.
EOF
```

Step 3: **Authentication (optional but recommended)**

If you use your website for file sharing, we strongly recommend you to set up password protection for your files. Please refer to the "Authentication" part of the instructions, located here:
https://labs.icahn.mssm.edu/minervalab/documentation/web-services/

Web Server

The ***indexes* option** is turned off by default for security reasons. You will an see error message "Forbidden, You don't have permission to access this resource." if you don't have an **index.html/ index.php** file under the folder.

You can enable this option in the htaccess file in order to list your files, for example:

```
[gail01@li03c03 ~]# cat /hpc/users/gail01/www/.htaccess
Options +Indexes
```

However, access to /sc and /hpc/users will be disabled around 1 Jan 2023. Alternate methods to publish data are being investigated.

Web server https://users.hpc.mssm.edu/

Some demos on setting up your first python flask and dash app

https://gail01.u.hpc.mssm.edu/flask_demo/

https://gail01.u.hpc.mssm.edu/dash_demo/

Code is at https://gail01.u.hpc.mssm.edu/code/

Load Sharing Facility(LSF)

A Distributed Resource Management System

bsub - submit a batch job to LSF

- command job submission: bsub [options] command

  $ bsub -P acc_hpcstaff -q premium-n 1 -W 00:10 echo "Hello Chimera"

- LSF script submission: bsub [options] < my_batch_job (Options on the command line override what is in the script)

```
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>.
```

LSF: batch job submission examples with bsub

Interactive session:

 # interactive session

$ bsub -P acc_hpcstaff -q interactive -n 1 -W 00:10 -Is /bin/bash

 # interactive GPU nodes, flag "-R v100" is required

$ bsub -P acc_hpcstaff -q interactive -n 1 -R v100 -gpu num=1 -R span[hosts=1] -W 01:00 -Is /bin/bash

Batch jobs submission:

 # simple standard job submission

$ bsub -P acc_hpcstaff -q premium-n 1 -W 00:10 echo "Hello World"

 # GPU job submission if you don't mind the GPU card model

$ bsub -P acc_hpcstaff -q gpu -n 1 -gpu num=1 -R span[hosts=1] -W 00:10 echo "Hello World"

*# himem job submission, flag "**-R himem**" is required*

*$ bsub -P acc_hpcstaff -q **premium** -n 1 -R himem -W 00:10 echo "Hello World"*

Last but not Least

Got a problem? Need a program installed? Send an email to:

hpchelp@hpc.mssm.edu