Introduction to Minerva

Minerva Scientific Computing Environment

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

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Icahn
School of
Medicine at
Mount
Sinai

Outlines

- Compute and storage resources
- Account and logging in
- User software environment
    - Lmod, anaconda, singularity, Jupyter, RStudio

Minerva cluster @ Mount Sinai

Chimera Partition:

- 4x **login nodes** - Intel Emerald Rapids 8568Y+, 2.3GHz – 96 cores with 512 GB memory per node.
- Compute nodes -
  - 146 **high memory nodes** - Intel Emerald Rapids 8568Y+, 2.3GHz - 96 cores with 1.5 TB memory per node.)
  - 37 **high memory nodes** - Intel 8168/8268, 2.7/2.9GHz - **1.5 TB** mem/node
  - **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
    - 2 - Intel 8358,2.6GHz - 2 TB memory - 4x A100- **80 GB** GPU
    - 2 - Intel 8358 2.6 GHz- 500 GB memory - 4x H100- **80 GB** GPU
    - 47 - Intel ER 8568Y+, 2.3GHz - 1.5 TB memory - 4x H100- **80 GB** GPU
    - 4 - AMD Genoa 9334 2.7GHz - 1.5 TB memory - 8x L40S- **48 GB** GPU

NIH FUNDED NODES

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: 32 PB 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**

General Minerva Information

- The Minerva website is:

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

  - 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 Rocky 9

- 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
  - Hospital user will need to request a “School Network Account” via SailPoint.
- Register your token at the Self Service Portal **school site** (https://register4vip.**mssm**.edu/vipssp/)
- Complete forms at https://forms.hpc.mssm.edu/ to activate your account after it is created.
- 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*

Annual Forms

- 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, the NIH acknowledgement, and MSHS AI Implementation and Use Policy, then sign all agreement forms **annually** (every Jan.) at

  https://forms.hpc.mssm.edu/

- Users who have not signed all agreements will have their accounts locked until all the agreements are signed.

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

```
[yuj25@li04e03 ~]$ minerva_help

Minerva HPC website:     https://labs.icahn.mssm.edu/minervalab/
Minerva Documentation at https://labs.icahn.mssm.edu/minervalab/documentation/
Minerva training slides at https://labs.icahn.mssm.edu/minervalab/resources/the-minerva-user-group-and-training-classes/

Publish R/shiny to Rstudio Connect server: https://labs.icahn.mssm.edu/minervalab/rstudio-connect-server/
Data transfer:                   https://labs.icahn.mssm.edu/minervalab/documentation/file-transfer-globus/
Web service:                     https://labs.icahn.mssm.edu/minervalab/documentation/web-services/
TSM data archive:                https://labs.icahn.mssm.edu/minervalab/documentation/access-tsm-with-command-line/

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-module.sh (with details at https://labs.icahn.mssm.edu/minervalab/documen
tation/r/)

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

Logging in - login nodes

4 login nodes: minerva[11-14], which points to the login node **li04e[01-04]**

- only available within campus-network

Users	Login method	Login servers	Password Components
Sinai users	userID	**@minerva.hpc.mssm.edu** **or specific nodes:** **@minerva11.hpc.mssm.edu** **@minerva12.hpc.mssm.edu** **@minerva13.hpc.mssm.edu** **@minerva14.hpc.mssm.edu**	Sinai Password followed by 6 Digit Symantec VIP token code
External users			

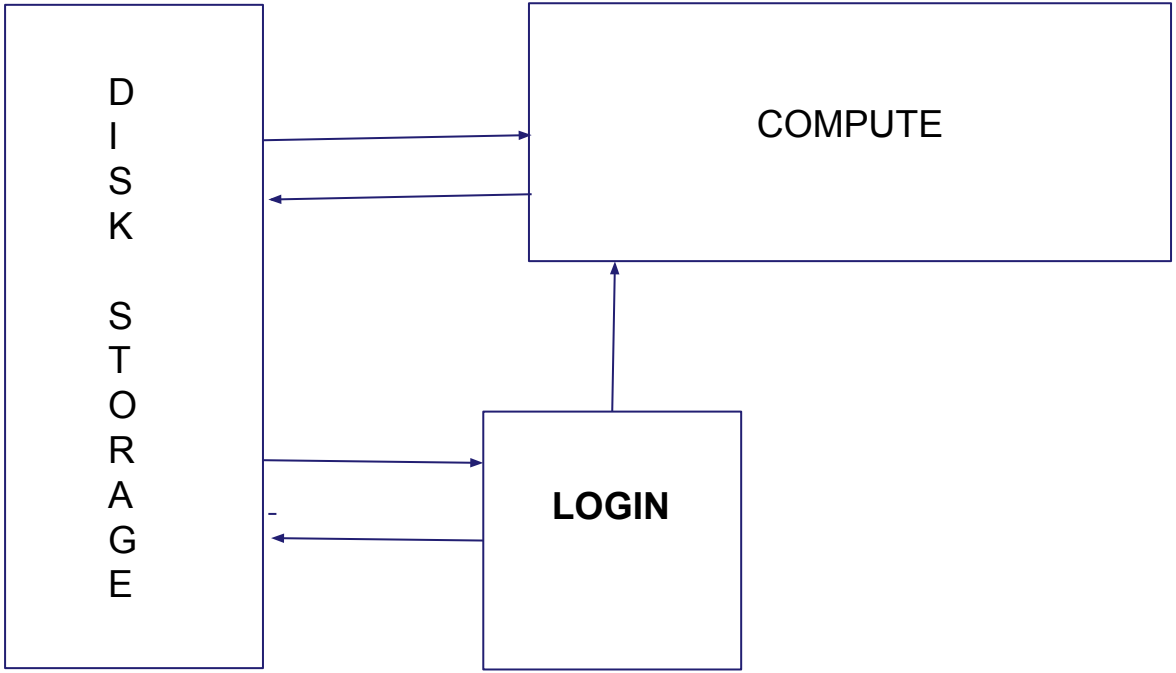
Note: Load balancer **Round-robin** is configured for **minerva.hpc.mssm.edu.** It will distribute client connections to the nearest across a group of login nodes.

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**	• 30GB 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 **$155**/TiB/yr

Minerva Cluster from 30,000 ft.



Minerva Ticket Submission

- Send an email to: hpchelp@hpc.mssm.edu to start a ticket.
- Information to include:
  - The error message or the location of the log file on Minerva.
    - use command “pwd” to check the current working directory.
  - All the commands you used to get the error message.
  - The location of the scripts used and how did you run the script.
  - Which node.
    - yuj25@li04e04
  - The job ID and location of the job script.
    - Job <123456789> is submitted to queue <premium>.

- Please do not include any “<” in the email.

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/4.2.0, R/4.4.1, ……
- To check the detailed PATH setting in module files: **$ml show R**
- Load module: **$ml python or $module load python** or **$ml python/3.12.5** (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:
  - Minerva Lmod guide
  - Lmod user guide

User Software Environment - Major packages

OS: **Rocky 9** with **glibc-2.34(GNU C library) available**

GCC: system default /usr/bin/gcc is gcc 11.4

$ module load gcc (default is 14.2.0) or *$ ml gcc*

$ ml python Python: default version 3.12.5 (it will load python and all available python packages)

$ ml R R: default version 4.2.0 (it will load R and all available R packages), more recent version 4.4.1

$ml CPAN Collection of system Perl software: default system version 5.40.0

$ml anaconda3 Anaconda3: default version 2024-06

$ml java java: latest version 21.0.4

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

- https://labs.icahn.mssm.edu/minervalab/documentation/conda/
- **To avoid incompatibilities with other python, clear your environment with module purge before loading Anaconda**

  $ml purge

  $ml anaconda3/2024.06

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

- 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/3.6.4*

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 sessions here

User Software - How to Run Jupyter Notebook

Option 1 : On-the-fly Jupyter Notebook in a Minerva job

https://labs.icahn.mssm.edu/minervalab/documentation/python-and-jupyter-notebook/#jupyter

- Scripts in /usr/local/bin on head nodes only:
  - (Not recommended) **`minerva-jupyter-web.sh`**
    - Runs jupyter installed inside a singularity container
    - No module system setup
  - **`minerva-jupyter-module-web.sh`**
    - Runs jupyter installed in module python/3.12.5
    - Can access modules on minerva
    - Can load users' conda environments (jupyter must be installed in conda env)
      - **`minerva-jupyter-module-web.sh -mm anaconda3/2024.06 -env ENV_NAME`**
      - Install jupyter in your conda env: ***`conda install jupyter`***
      - Do not have any conda env activated before running the script.
- Add --help to the script to get help message/usage

User Software - How to Run Jupyter Notebook

Option 2 : Jupyter Notebook in a batch job

- Primarily, the nbconvert tool allows you to convert a Jupyter .ipynb notebook document file into another static format including HTML, LaTeX, PDF, Markdown, reStructuredText, and more. nbconvert can also add productivity to your workflow when used to execute notebooks programmatically.
  https://nbconvert.readthedocs.io/en/latest/usage.html
- Use the commands below in your job script:

```
ml python/3.12.5
jupyter nbconvert --to notebook --execute myfile.ipynb
```

- The result is saved in a file named **myfile.nbconvert.ipynb**

Option 3 : Via Open Ondemand

User Software - Rstudio

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

https://labs.icahn.mssm.edu/minervalab/documentation/r/#rstudio

- Scripts in /usr/local/bin on login nodes only:
  - (Not recommended) Scripts run RStudio Server installed inside singularity containers, no module system setup:
    - **`minerva-rstudio-web-r4.sh`**
    - **`minerva-rstudio-web-r4.2.3.sh`**
  - Scripts with module system setup:
    - **`minerva-rstudio-web-module.sh`**
- Add --help to the script to get help message/usage

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

- Enable X11 forwarding
- Run "`ml rstudio proxies; rstudio`"

Option 3 : Via Open Ondemand

Next session: Essential Services on Minerva Friday, September 19, 2025

- Posit Connect
- File Transfer - Globus
- Archiving Data: IBM Tivoli Storage Management (TSM)
- Web server

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Last but not Least

Got a problem? Send an email to:

hpchelp@hpc.mssm.edu