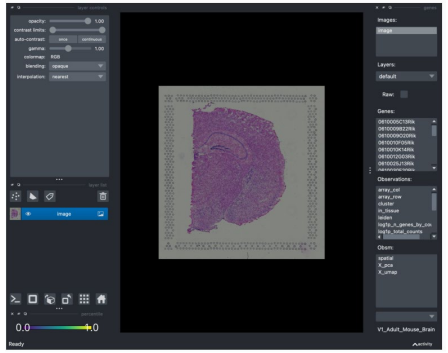
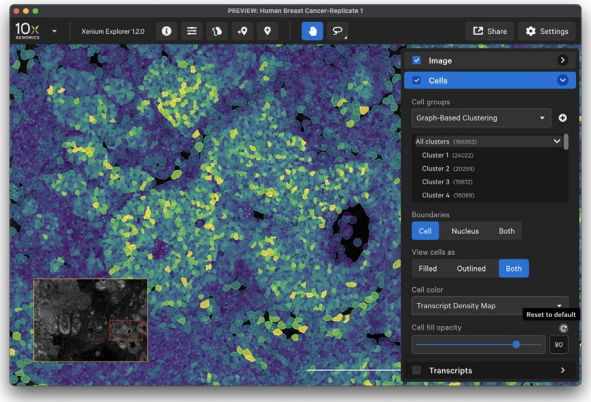
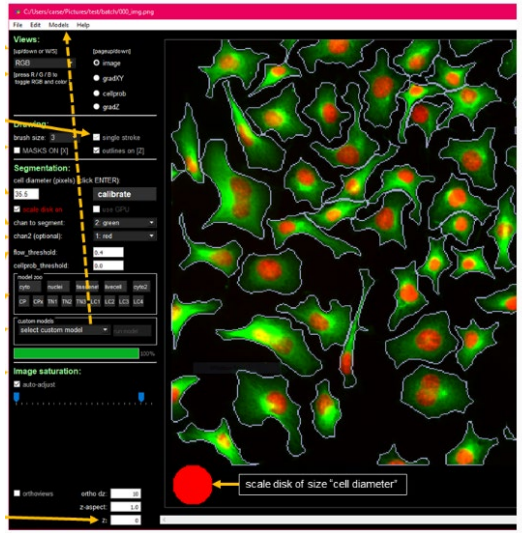
Interactive Computing on the HPC3 for Spatial-omics







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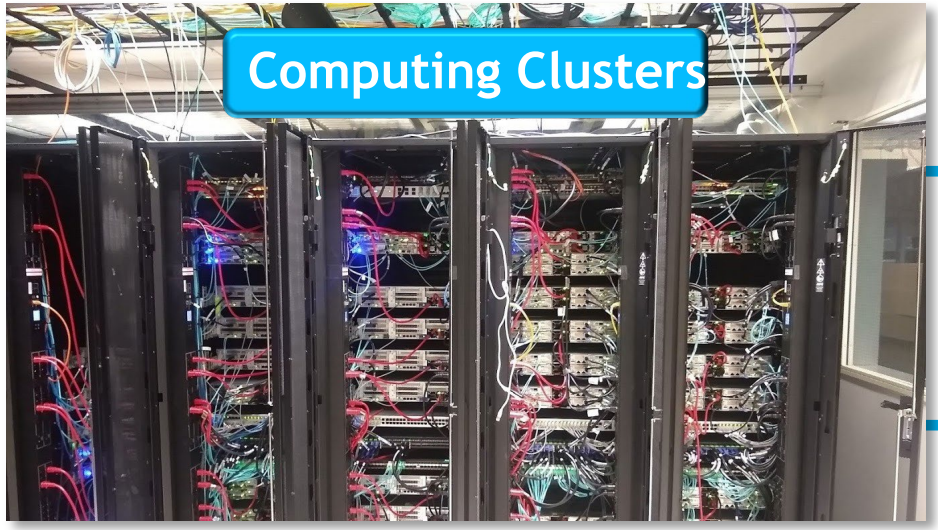
Workshop Agenda

- **Overview of HPC3**
  - Connecting to HPC3 & loading software modules
  - Navigating file systems and managing storage
  - Slurm account management and sample job submission
- Interactive Computing on HPC3
  - SSH x11 forwarding/tunneling of software
  - Containers on HPC3 and Jupyter Eco System
  - Jupyter notebook and JupyterLab
  - RStudios and RShiny Apps
  - XPRA x11 to HTML5 via Jupyterhub
- Spatial-omics Apps (Live Demo)
  - Fiji & CellProfiler
  - Loupe Browser & Xenium Explorer
  - CellPose & SquidPy

Overview of HPC3

The rest of the slide deck are for your reference only. We will not be going through these directly for this workshop.

Key UCI HPC3 Resource Specs



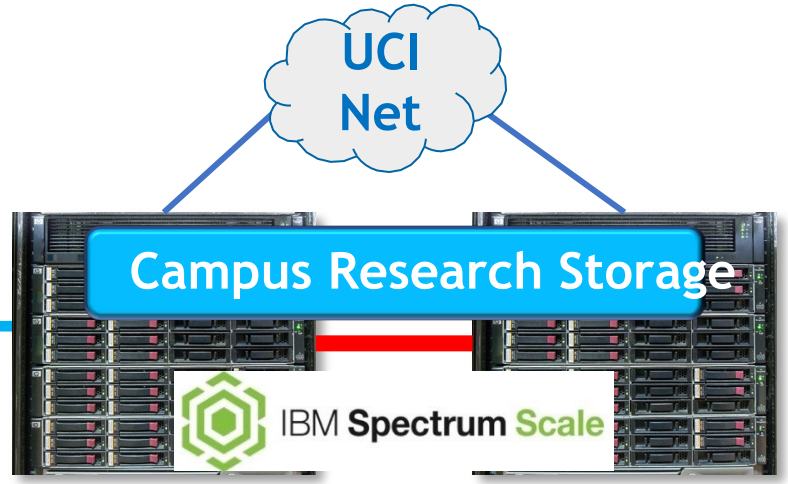
HPC3 - Rocky 8.8 Linux Distro

- ~9400 Cores/216 Hosts (compute nodes)
- 57,846 GB Aggregated memory
- 52 Nvidia V100 16Gb GPUs
- 56 Nvidia A30 24GB GPUs
- 8 Nvidia A100 80GB GPUs
- EDR (100Gbps) Infiniband
- 10GbE Ethernet
- Minimum
  - 4GB memory/core
  - AVX2 instruction set (Epyc/Intel CPUs)

Eight Parallel File Systems

DFS3, DFS4, DFS5, …

- 7PB usable storage
- ~6GB/sec bandwidth/System
- Single Copy/No Snapshots



CRSP – Campus Research Storage Pool

- 1 PB usable storage
- Available anywhere on UCI Network
- Dual Copy of All Data
- Snapshots
- Highly available

https://rcic.uci.edu/hpc3/specs.html

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HPC3 Quick Start Guides

(https://rcic.uci.edu/about/intro.html)

Getting an account	send email to **hpc-support@uci.edu**
Logging in	**Connecting to HPC3**
Submitting your first job	**SLURM tutorial**
Available software	**Environment modules tutorial**
Purchasing Hardware/Core Hours	**Beyond baseline allocation**
All about accounting	**Free and Accounted jobs**
Storage	**Home Area, Parallel File Systems, and CRSP**
Getting Help	**Ask for help or software install**

Basics of being a good citizen on a cluster

1. Cluster is a shared resource, it is NOT your personal machine
2. What you do affects all the other users, so think before you hit that *Enter* key
   - Do not run interactive jobs on login nodes
   - Do not transfer data on login nodes
3. Secured from mischief and disasters.
   - We restrict users' ability (permissions) to install and run unwanted software applications
   - It is your responsibility to act secure
   - Be careful when bringing applications from unknown sources. DO NOT ask for sudo access
4. For your jobs: use resources you need, don't ask for more

   Study this Slurm guide https://rcic.uci.edu/slurm/slurm.html
5. Be mindful how you submit tickets

   Getting help!

High-level View of what things cost

No Cost Allocations

Role	HPC3 Core Hours	GPU Hours	Home Area Storage	DFS Storage	CRSP Storage
Faculty	200K hours/year[1]	By Request ~2K hours/year[1]	50GB	1TB in Pub	1 TB
Student	1000 hours	---	50GB	1TB in Pub	---

Cloud-like Costs

	HPC3 Core Hours	GPU Hours	Home Area Storage	DFS Storage	CRSP Storage
Faculty	$.01/core hour	$0.32/GPU hour	Not expandable	$100/TB/5 years	$60/TB/year
AWS Equivalent	C5n.large $.063	P3.2xlarge $1.95	---	---	S3[2] Standard $242/TB/year

[1] Exact amounts dependent on # requests/available hardware

[2] Comparison difficult - S3 has higher durability, CRSP has no networking fee.

HPC3 Policies for CPU and memory scheduling

Partition	Default memory/core	Max memory/core	Default / Max runtime	Cost	Jobs preemption
CPU Partitions					
standard	3 GB	6 GB	2 day / 14 day	1 / core-hr	No
free	3 GB	18 GB	1 day / 3 day	0	Yes
debug	3 GB	18 GB	15 min / 30 min	1 / core-hr	No
highmem	6 GB	10 GB	2 day / 14 day	1 / core-hr	No
hugemem	18 GB	18 GB	2 day / 14 day	1 / core-hr	No
maxmem	1.5 TB/node	1.5 TB/node	1 day / 7 day	40 / node-hr	No
GPU Partitions					
gpu3	3 GB	9 GB	2 day / 14 day	1 / core-hr, 32 / GPU-hr	No
free-gpu	3 GB	9 GB	1 day / 3 day	0	Yes
gpu-debug	3 GB	9 GB	15 min / 30 min	1 / core-hr, 32 / GPU-hr	No

RCIC Recommended Online Tutorials

The Missing Semester of Your CS Education Many topics as separate lectures, including Shell Tools and Scripting, Editors (Vim), Command-line Environment, Data Wrangling, Git, security and more.

The Software Carpentry teaches basic skills via workshops and lessons, here are direct links:

- **The UNIX Shell** The Unix shell fundamentals
- **Introduction to Python** Learn the basics of Python programming language.
- **Introduction to R** Learn the basics of R programming language.

Connecting to HPC3 and loading software modules

Logging onto HPC3

Step 1 Connect to UCI campus VPN, see instructions **UCI campus VPN**

Step 2 Open your Terminal application and start ssh session. Alternatively, you could use the jupyterhub interface at https://hpc3.rcic.uci.edu/biojhub4/ directly in your browser

Step 3 Either in ssh session or jupyterhub interface, you will need to use your regular UCI credentials (UCINetID and password) to connect to an HPC3 login node **hpc3.rcic.uci.edu**

SSH login Example

- Logging in is via ssh with your UCInetID
  ssh hpc3.rcic.uci.edu **-l panteater**
  or
  ssh **panteater@hpc3.rcic.uci.edu**
- Use passphrase and ssh public key authentication Do not use empty ssh passphrase!!! https://www.ssh.com/ssh/public-key-authentication
- If you plan to run interactive graphics programs
  ssh -X -Y hpc3.rcic.uci.edu -l panteater

  But X11 used by Linux for graphics is high bandwidth and can be sensitive to network latency, some people prefer **x2go**
  https://wiki.x2go.org/doku.php

Duo authentication

Password:
Duo two-factor login for <UCINETID>

Enter a passcode or select one of the following options:

1. Duo Push to XXX-XXX-XXXX

Passcode or option (1-1):

After a successful login you will see a screen similar to the following:

```
Last login: Thu Jul 15 15:25:59 2021 from 10.240.58.4
+-----------------------------------------+
|  _                 _                _ _ _____   |
| | | ____   __ _(_)_ __         (_) | ___|  |
| | |/ _ \ / _` | | '_ \ _____| | |___ \  |
| | | (_) | (_| | | | | |_____| | |___) | |
| |_|\___/ \__, |_|_| |_|     |_|_|____/  |
|           |___/                         |
+-----------------------------------------+
 Distro:  Rocky 8.8 Core
 Virtual: NO

 CPUs:    40
 RAM:     191.9GB
 BUILT:   2023-03-02 13:32

 ACCEPTABLE USE: https://rcic.uci.edu/documents/RCIC-Acceptable-Use-Policy.pdf
  login-i15 2001%
```

Loading software modules

- **Environment module** is a user interface to the Modules package which provides for the dynamic modification of the user's environment via modulefiles.
- Each **modulefile** contains all the info needed to configure the shell to use a specific application.
- Command **module load** interprets the modulefiles and
  - Sets aliases
  - Sets environment variables
  - Loads depended modules
- Command **module avail** lists all installed software and their versions

General info for Linux https://modules.readthedocs.io/en/latest/
Read User guide for HPC3 https://rcic.uci.edu/software/modules.html

Environment modules update your environment

Case 1: usage of multiple versions of software

```
login-i16 which R
/usr/bin/which: no R in (/usr/local/bin:/usr/bin:/usr/sbin:/data/homezvol0/npw/bin)
login-i16 module avail R
---------- /opt/rcic/Modules/modulefiles/LANGUAGES -------
R/3.6.2 R/4.0.2
login-i16 module load R/4.0.2
login-i16 which R
/opt/apps/R/4.0.2/bin/R
login-i16 module list
Currently Loaded Modulefiles:

1) OpenBLAS/0.3.6          2) java/1.8.0       3)
icu/65.1  login-i16 module unload R/4.0.2
login-i16 module list
No Modulefiles Currently Loaded.
login-i16 module load R/3.6.2
login-i16 which R
/opt/apps/R/3.6.2/bin/R
```

Case 2: load/unload different software modules

```
login-i16 module load gcc/8.4.0
login-i16 module list
Currently Loaded Modulefiles:
  1) gcc/8.4.0
login-i16 module load hdf5/1.10.5/gcc.8.4.0
login-i16 module list
Currently Loaded Modulefiles:
  1) gcc/8.4.0       2) java/1.8.0       3) hdf5/1.10.5/gcc.8.4
login-i16 module unload hdf5/1.10.5/gcc.8.4.0
login-i16 module list
Currently Loaded Modulefiles:
  1) gcc/8.4.0
```

Always unload module in reverse order: FILO!

Environment module commands summary

search

```
$ module avail
```
shows all installed software environment

```
$ module avail R
```
modules show R modules

```
$ module keyword salmon
```
check all modules for a keyword

```
salmon/1.1.0        : Name__salmon
salmon/1.1.0        :
```

info

```
$ module display R
```
shows environment modification + description

```
$ module help R
```
show module specific help (description)

use

```
$ module load R
```
loads R at whatever latest version not ideal

```
$ module load R/4.0.2
```
loads R at specified version preferred method

```
$ module list
```
lists currently loaded modules

```
$ module unload R/4.0.2
```
unloads specified module (in reverse order if many)

```
$ module purge
```
removes all loaded modules

Navigating file systems and managing storage

The filesystem storage is generally in 3 areas. Please see the links below for detailed information about each filesystem.

HOME	**The HOME area** has a 50GB quota for each user. In addition, there is a space for snapshots. Total for home and snapshots is 100GB. Each user HOME is in /data/homezvolX/<account>
DFS	**The BeeGFS Parallel storage File System (DFS)** access remains the same. All users have /pub/<account> area. Depending on a lab affiliation, users may have space in /dfs3, /dfs4, /dfs5, /dfs6, /dfs7, /dfs8, /dfs9 (9/19/2023)
CRSP	**The Campus Research Storage Pool (CRSP)** is available in /share/crsp. Depending on a lab affiliation, users may have space in /share/crsp/lab/<labname./<account>

Check $HOME quota

To see your current quota usage do:

```
[user@login-x:~]$ df -h ~
Filesystem                          Size  Used Avail Use% Mounted on
 10.240.58.6:/homezvol0/panteater   50G  3.5G   47G   7% /data/homezvol0/panteater
```

The **~** stands for your $HOME. The output above shows that user panteater used 3.5Gb of its 50Gb allocation.

If you want to see the usage by files and directories in $HOME

```
[user@login-x:~]$ cd
[user@login-x:~]$ ls
bin                 examples     local         perl5
biojhub3_dir        info         mat.yaml      R
classify-image.py   keras-nn.py  modulefiles   sbank-out

[user@login-x:~]$ du -s -h *
7.0M    bin
166M    biojhub3_dir
8.5K    classify-image.py
647K    examples
91K     info
4.5K    keras-nn.py
126M    local
4.5K    mat.yaml
60K     modulefiles
512     perl5
1.2G    R
 25K    sbank-out
```

	change to your $HOME directory
	list contents of $HOME
	find disk usage for each file and directory in $HOME. The output shows disk usage in kilobytes (K), megabytes (M) or gigabytes (G). For directories, all contents inside are included. For example, a directory **R** uses 1.2Gb of disk space.

To see the quotas for user panteater on DFS pool /dfs6

```
[user@login-x:~]$ dfsquotas panteater dfs6
==== [Group Quotas on dfs6]

Quota information for storage pool Default (ID: 1):

      user/group     ||            size            ||    chunk files
     name      |  id  ||    used    |    hard    ||  used   |  hard
---------------|------||------------|------------||---------|---------
 panteater_lab|012345||   26.25 TiB|   50.00 TiB||  1310459| 18500000
   alpha_users|158537||      0 Byte|      1 Byte||        0|        1
      panteater|000865||  755.59 GiB| 1024.00 GiB||   258856|unlimited
```

Data Transfer to HPC3

Often users need to brings data from other servers and laptops. To transfer data one needs to use `scp` (secure copy) or `rsync` (file copying tool). Please see **detailed data transfer examples**. Alternatively, one can use graphical tools (Filezilla, MountainDuck, or WinSCP) to transfer files between a local laptop and the cluster. Follow each program instructions how to do this.

In all of the transfer application you will need to use hpc3.rcic.uci.edu to indicate a remote server (where you want to transfer your files) and use your UCNetID credentials for your user name and password.

Slurm account management and sample job submission

HPC3 SLURM

Slurm is an open-source workload manager for Linux clusters and provides:

1. access to resources (computer nodes) to users so they can run their applications.
2. framework to start, execute, and monitor work on a set of allocated nodes.
3. management of a queue for pending work.

Helpful UCI HPC3 specific slurm guide:

https://rcic.uci.edu/hpc3/slurm.html

Simple code of conduct for running applications on HPC3

1. **All jobs, batch or interactive must be submitted to the scheduler**
2. **Do not run computational jobs on login nodes** this adversely affects many users. Login nodes are meant for light editing or compilation and for submitting jobs. Any job that runs for more than an hour or is using significant memory and CPU within an hour should be submitted to Slurm either as interactive or batch job.
3. **Ssh access to the compute nodes is turned off** to prevent users from starting jobs bypassing Slurm. See **attaching to running job** below.
4. **Do not run Slurm jobs in your $HOME**.
5. **Make sure you stay within your disk quota**. File system limits are generally the first ones that will negatively affect your job. See **storage guides**

Cluster Partitions

HPC3 has different kinds of hardware, memory footprints, and nodes with GPUs. All nodes (servers) all are separated into groups according to their resources. Slurm uses the term partition to signify a queue of resources. We have a few separate partitions, most users will need to use *standard* and *free* partitions:

- **standard partition** is for jobs that should not be interrupted. Usage is charged against the user's Slurm bank account. Each user gets FREE one time allocation of 1000 core hours to run jobs here. **Users are NOT CHARGED ANY $**. If all allocation is used, users can run jobs only if they are associated with labs that have core hours in their lab banks. Usually, lab bank is a PI lab account.
- **free partition** is for jobs that can be preempted (killed) by standard jobs. Users can run jobs in this partition even if they have only 1 core-hour left. There are no charges for this partition.

HPC3 Policies for CPU and memory scheduling

Partition	Default memory/core	Max memory/core	Default / Max runtime	Cost	Jobs preemption
CPU Partitions					
standard	3GB	6GB	2day / 14day	1 / core-hr	No
free	3GB	18GB	1day / 3day	0	Yes
debug	3GB	18GB	15min / 30min	1/core-hr	No
highmem	6GB	10GB	2day / 14day	1/core-hr	No
hugemem	18GB	18GB	2day / 14day	1/core-hr	No
GPU Partitions					
gpu	3GB	9GB	2day / 14day	1/core-hr, 32/GPU-hr	No
free-gpu	3GB	9GB	1day / 3day	0	Yes
gpu-debug	3GB	9GB	15min / 30min	1/core-hr, 32/GPU-hr	No

Checking your allocations

`sbank` is short for "Slurm Bank". `Sbank` is used to display HPC3 user account information. In order to run jobs on HPC3, a user must have available CPU hours. To check how many CPU hours are available in your personal account, run the command with your account name:

```
[user@login-x:~]$ sbank balance statement -a panteater
User            Usage |         Account     Usage | Account Limit Available (CPU hrs)
---------- --------- + -------------- --------- + ------------- ---------
 panteater*         58 |       PANTEATER         58 |         1,000       942
```

To check how many CPU hours are available in all accounts that you have access to and how much you used:

```
[user@login-x:~]$ sbank balance statement -u panteater
User            Usage |         Account     Usage | Account Limit Available (CPU hrs)
User            Usage |         Account     Usage | Account Limit Available (CPU hrs)
---------- --------- + -------------- --------- + ------------- ---------
panteater*         58 |       PANTEATER         58 |         1,000       942
 panteater*      6,898 |          PI_LAB      6,898 |       100,000    93,102
```

Slurm Batch Job

simplejob.sub

```
#!/bin/bash

#SBATCH --job-name=test       ## Name of the job.
#SBATCH -A panteater_lab      ## account to charge
#SBATCH -p standard           ## partition/queue name
#SBATCH --nodes=1             ## (-N) number of nodes to use
#SBATCH --ntasks=1            ## (-n) number of tasks to launch
#SBATCH --cpus-per-task=1     ## number of cores the job needs
#SBATCH --error=slurm-%J.err ## error log file

# Run command hostname and save output to the file out.txt
  srun hostname > out.txt
```

To submit the job do:

```
[user@login-x:~]$ sbatch simplejob.sub
  Submitted batch job 362
```

Please look through https://rcic.uci.edu/hpc3/examples.html for different job examples

Job status

To check the status of your job in the queue:

```
[user@login-x:~]$ squeue -u panteater
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
               362  standard     test panteater R       0:03      1 hpc3-17-11
```

To get detailed info about the job:

```
[user@login-x:~]$ scontrol show job 362
```

The output will contain a list of key=value pairs that provide job information.

To cancel a specific job:

```
[user@login-x:~]$ scancel <jobid>
```

Job history

We have a cluster-specific tool to print a ledger of jobs based on specified arguments. Default is to print jobs of the current user for the last 30 days:

```
[user@login-x:~]$ /pub/hpc3/zotledger -u panteater
      DATE       USER    ACCOUNT PARTITION    JOBID  JOBNAME ARRAYLEN CPUS WALLHOURS     SUs
2021-07-21  panteater  panteater  standard  1740043     srun        -    1      0.00    0.00
2021-07-21  panteater  panteater  standard  1740054     bash        -    1      0.00    0.00
2021-08-03  panteater     lab021  standard  1406123     srun        -    1      0.05    0.05
2021-08-03  panteater     lab021  standard  1406130     srun        -    4      0.01    0.02
2021-08-03  panteater     lab021  standard  1406131     srun        -    4      0.01    0.02
    TOTALS          -          -         -         -        -    -      0.07    0.09
```

To find all available arguments use:

```
[user@login-x:~]$ /pub/hpc3/zotledger -h
```

Job info

`sacct` can be used to see accounting data for all jobs and job steps. An example below shows how to use job ID for the command:

```
[user@login-x:~]$ sacct -j 43223
       JobID  JobName  Partition      Account  AllocCPUS      State ExitCode
------------ -------- ---------- ------------ ---------- ---------- --------
   36811_374    array   standard panteater_l+          1  COMPLETED      0:0
```

The above command uses a default output format. A more useful example will set a specific format for sacct that provides extra information:

```
[user@login-x:~]$ export
SACCT_FORMAT="JobID%20,JobName,Partition,Elapsed,State,MaxRSS,AllocTRES%32"
[user@login-x:~]$ sacct -j 600
     JobID JobName  Partition  Elapsed     State  MaxRSS AllocTRES
---------- -------  --------  -------- --------- ------- --------------------------------
       600    all1  free-gpu  03:14:42 COMPLETED         billing=2,cpu=2,gres/gpu=1,mem=+
 600.batch   batch            03:14:42 COMPLETED 553856K           cpu=2,mem=6000M,node=1
 600.extern  extern             03:14:42 COMPLETED       0 billing=2,cpu=2,gres/gpu=1,mem=+
```

Interactive Computing

Slurm interactive jobs

To request an interactive job, use the `srun` command. Suppose you are enabled to charge to the panteater_lab account then, to start an interactive session you can use one of 3 methods :

```
[user@login-x:~]$ srun --pty /bin/bash -i                    (1)
[user@login-x:~]$ srun --pty -p free /bin/bash -i            (2)
[user@login-x:~]$ srun -A panteater_lab --pty /bin/bash -i   (3)
```

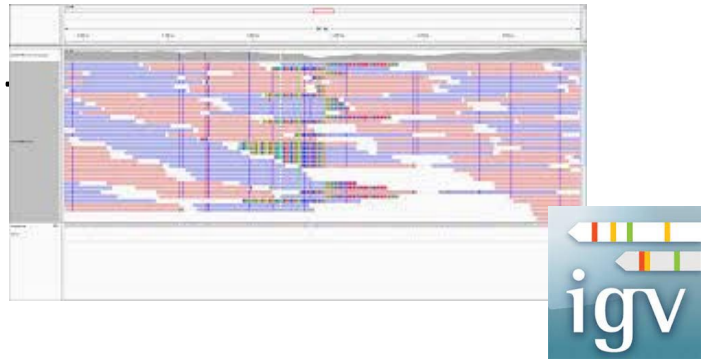
After you are done use `logout` command to logout:

```
[user@hpc3-l18-04:~]$ logout
```

	1) you will be put on an available node in standard partition using your default Slurm bank account
	2) you will be put on an available node in free partition using your default Slurm bank account
	3) you will be put on an available node in standard partition using panteater_lab account See 2.4. Interactive Job of https://rcic.uci.edu/hpc3/slurm.html for more options

Running Native X11 GUI apps

- Enable X11 forwarding in your SSH client
- For example: *ssh hpc3.rcic.uci.edu -X*
- Request an interactive session:
  - *srun -A account_lab -p standard --ntasks=1 --cpus-per-task=4 --nodes=1 --x11 --pty /bin/bash -i*
- Load application module (e.g. IGV Viewer)
  - *module load igv*
  - *Igv*
- X11 Application forwarded to your compu



Jupyter Ecosystem - Running Containers Interactively on HPC3

HPC3 User Authentication

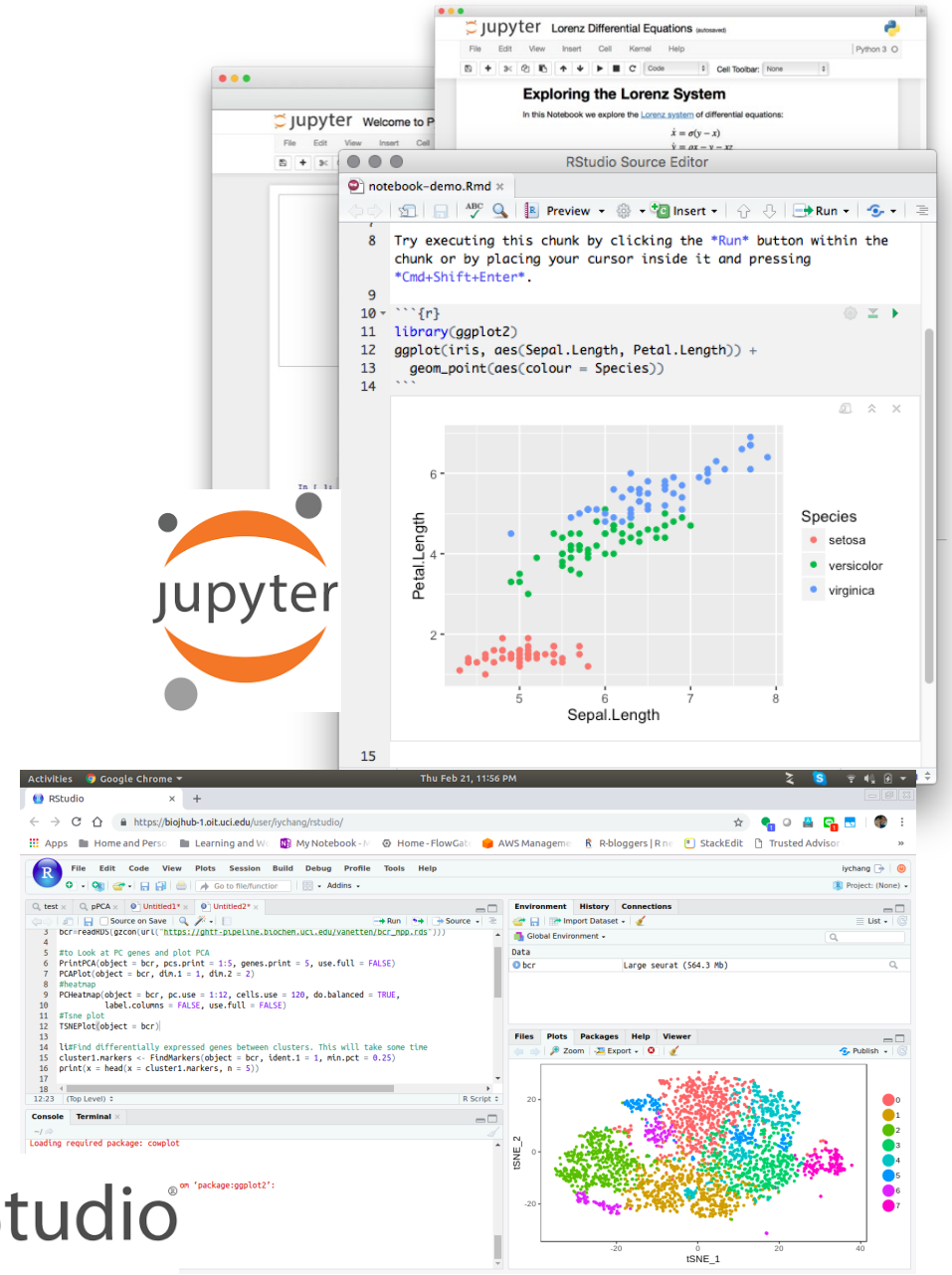
https://hpc3.rcic.uci.edu/biojhub3/

jupyterhub

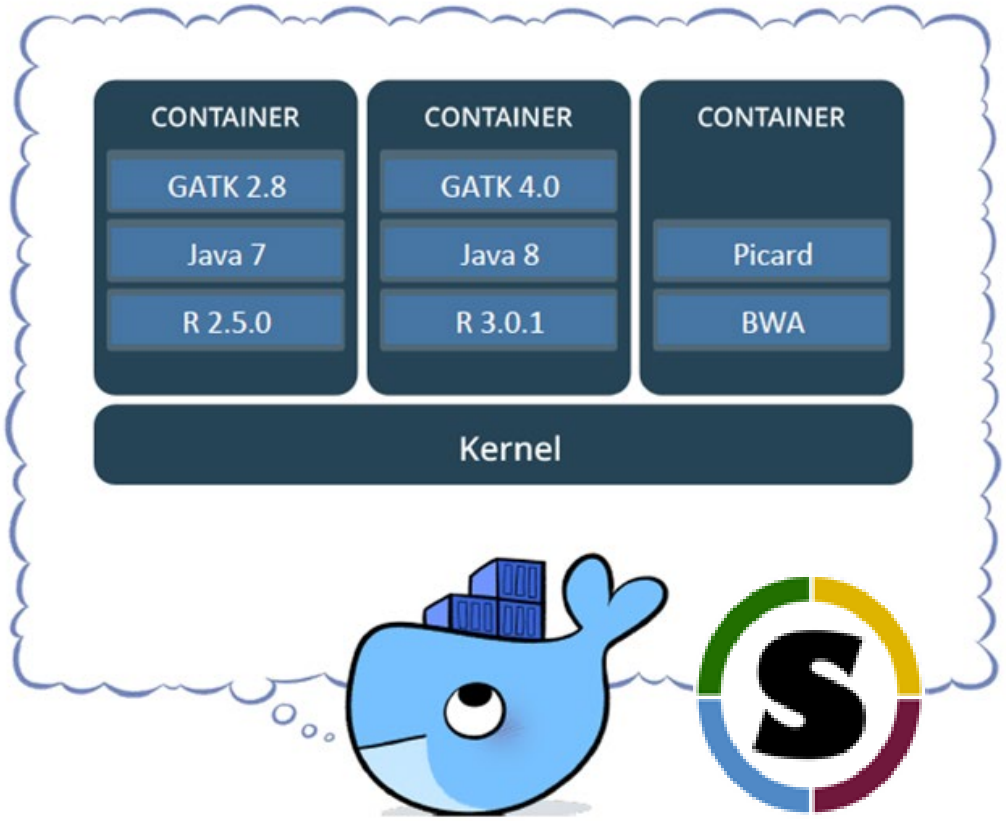
Container Selection

- Seurat2
- Seurat3
- ScanPy
- CellXGene

. . .



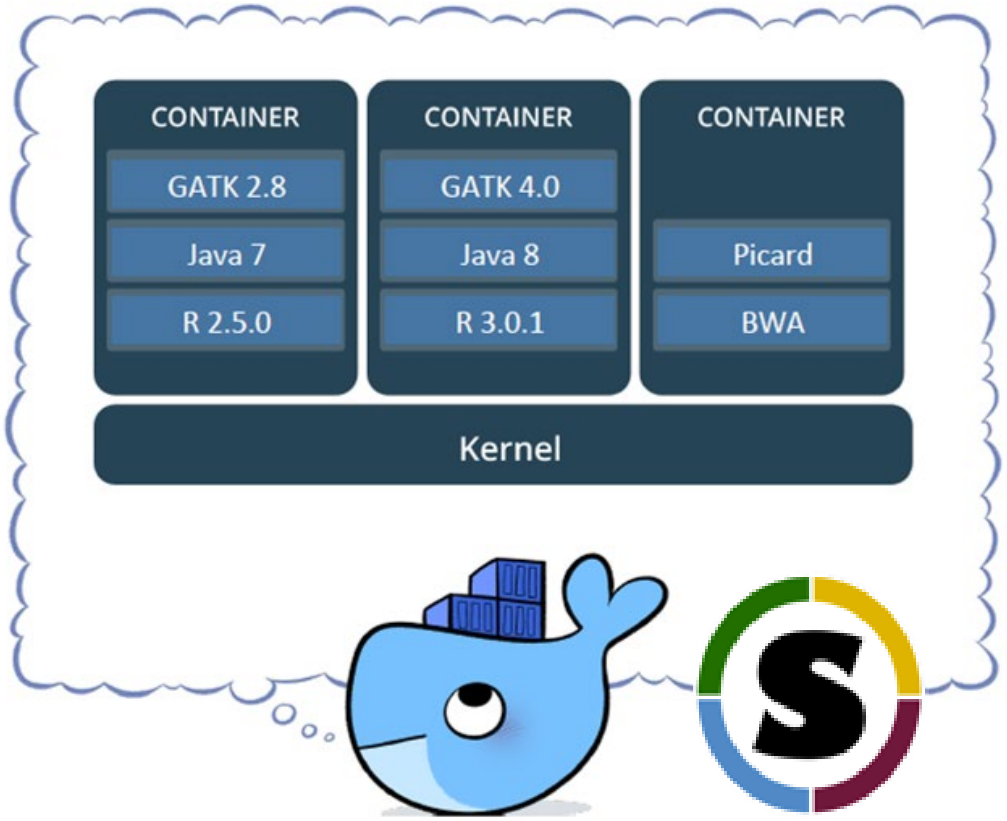
Container Technology Overview



Modified from https://www.docker.com/what-container

- Containers are isolated, but share OS and bins/libraries
- Provide highly customized software environment apart from the host system

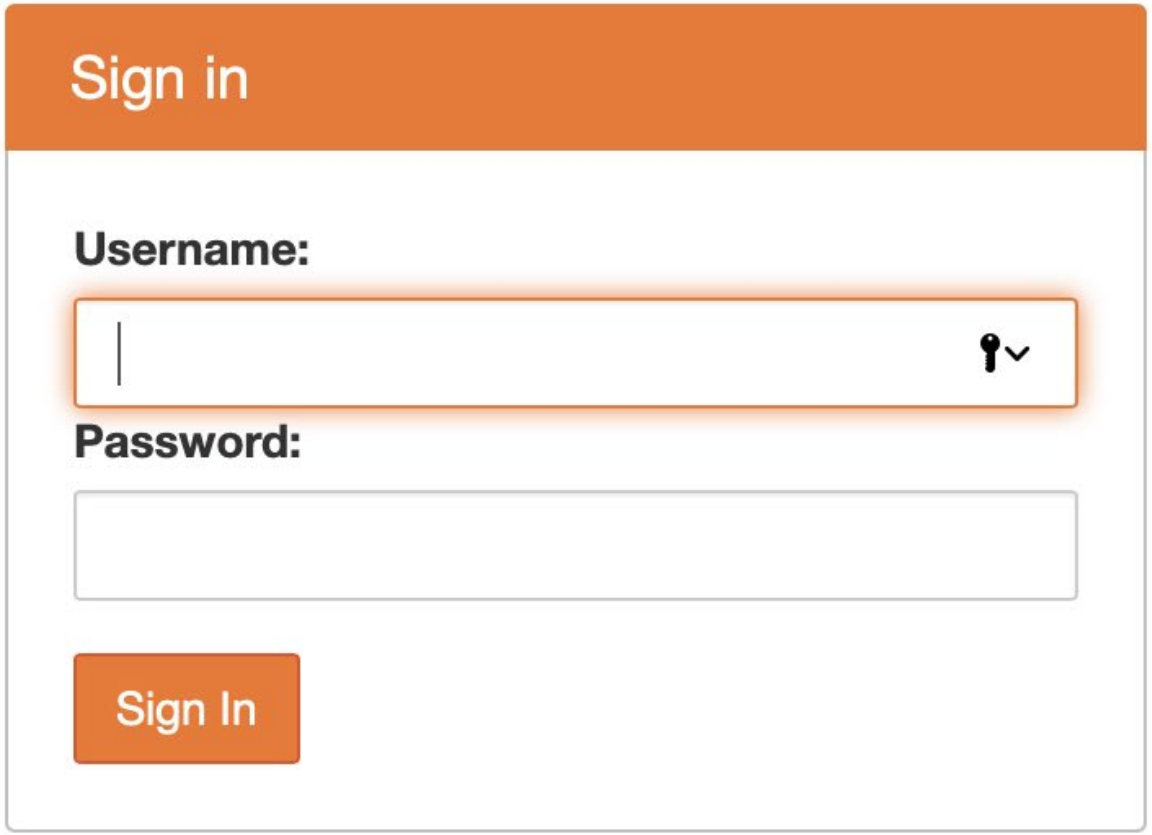
Container Benefits



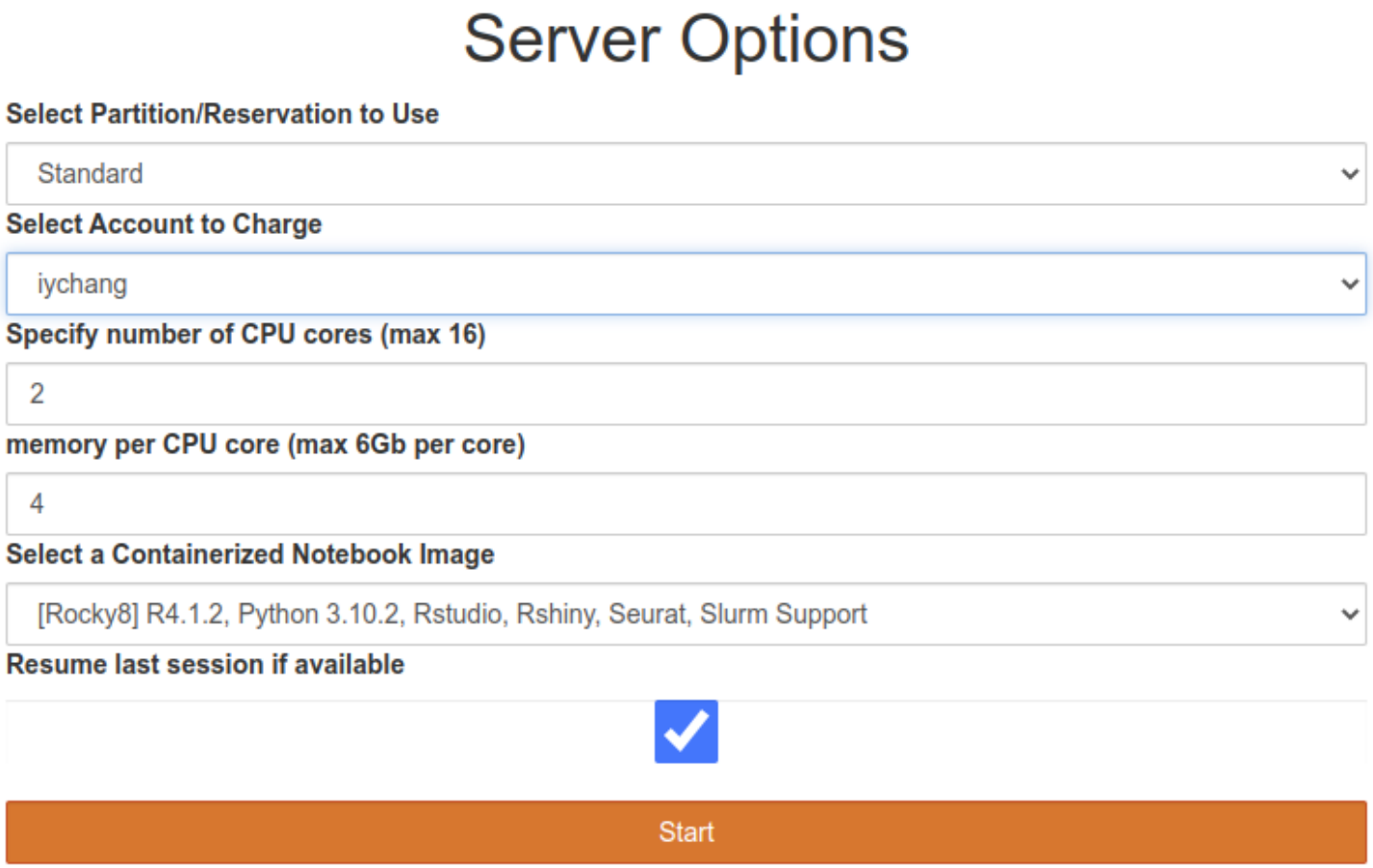
Modified from https://www.docker.com/what-container

- **Portability**: containers can be published and shared via cloud-based container hubs (https://hub.docker.com/, https://dockstore.org/, https://www.singularity-hub.org/) or transferred directly as image files
- **Versioning**: container build files can be stored in git/github repositories
- **Reproducibility**: published containers are immutable, and provides a snapshot of the computing environment used to run analysis

Using your favorite browser go to: https://hpc3.rcic.uci.edu/biojhub4/hub/login You will see the following screen where you will Use your usual HPC3 credentials to sign in:

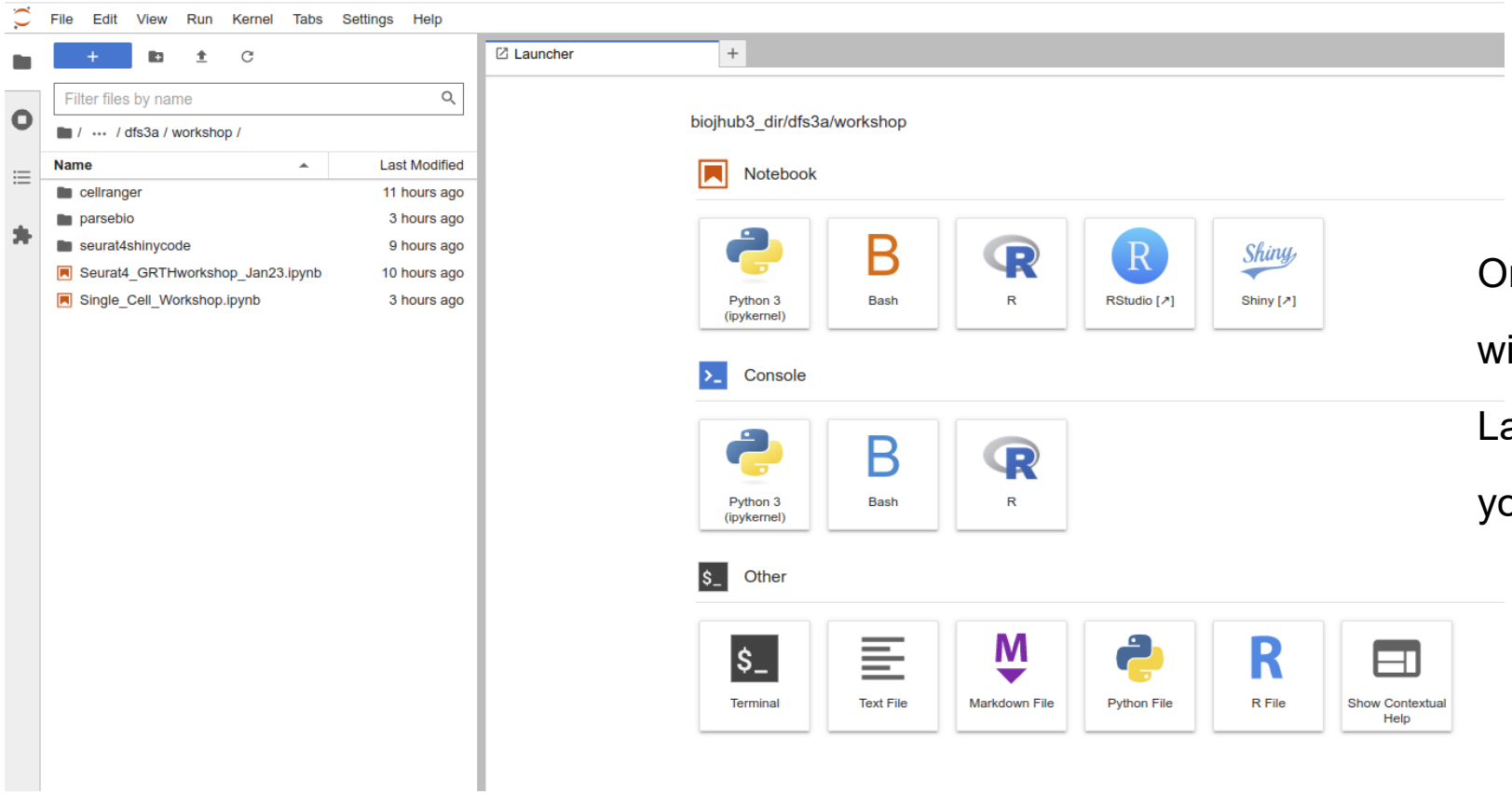


After authentication you will see a screen with server options as in the figure below:



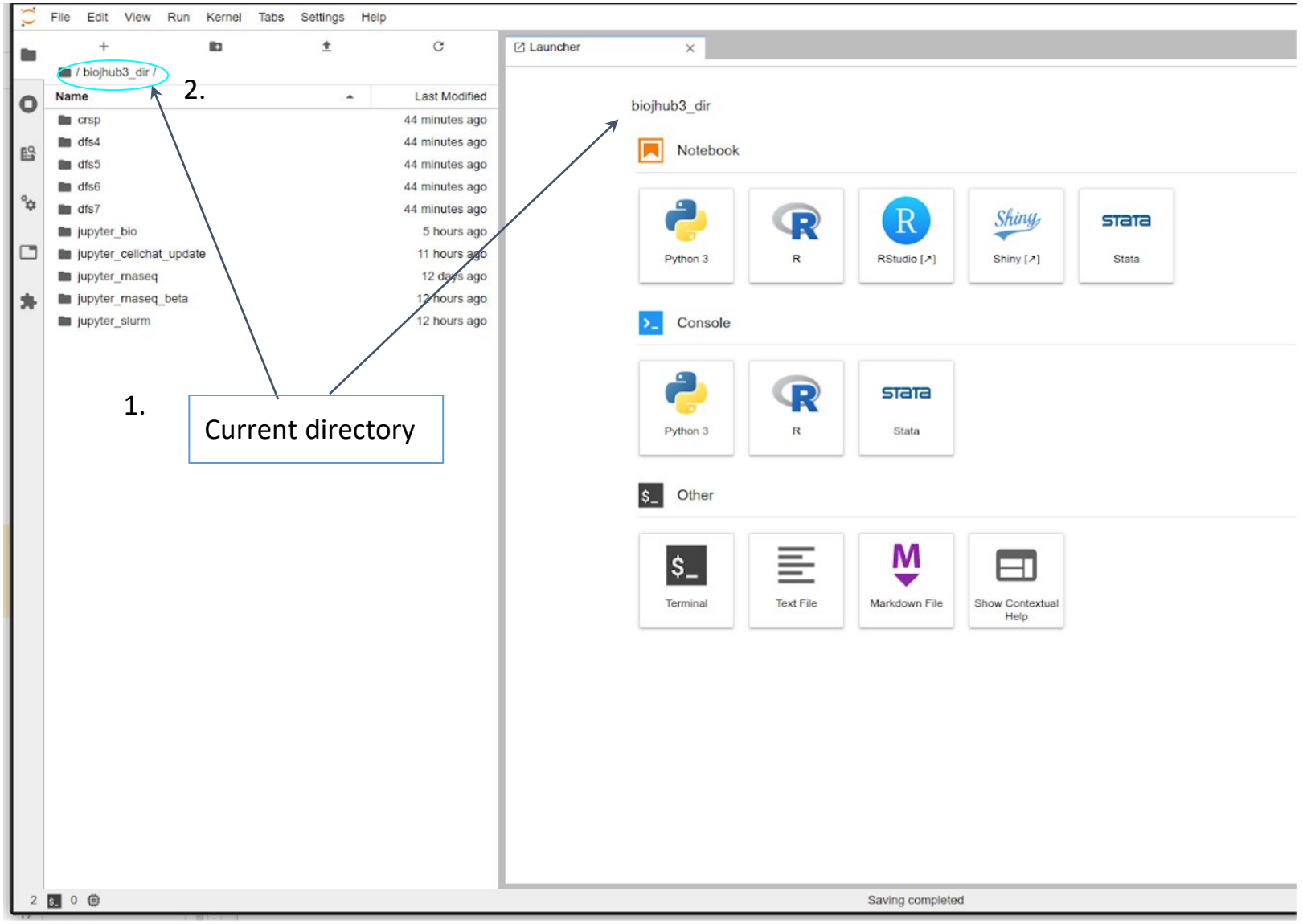
For this workshop, modify the *Select Account to Charge* to be one of your Slurm accounts, change number of CPUs to 4, select the "[Rocky8][Debug] Xpra Cellpose" container and press `Start`.

Main Jupyter Interface



Once the notebook is done spawning, you will get a file browser on the left, and a Launcher screen with a number GUI apps you can use on the right.

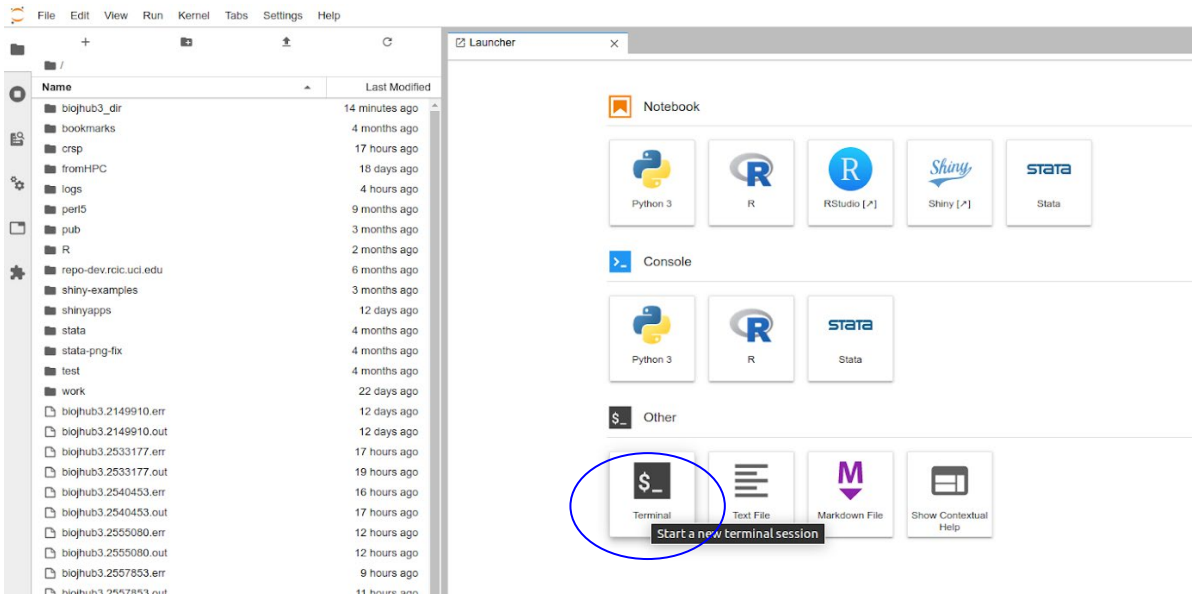
Navigating File Systems in Jupyter

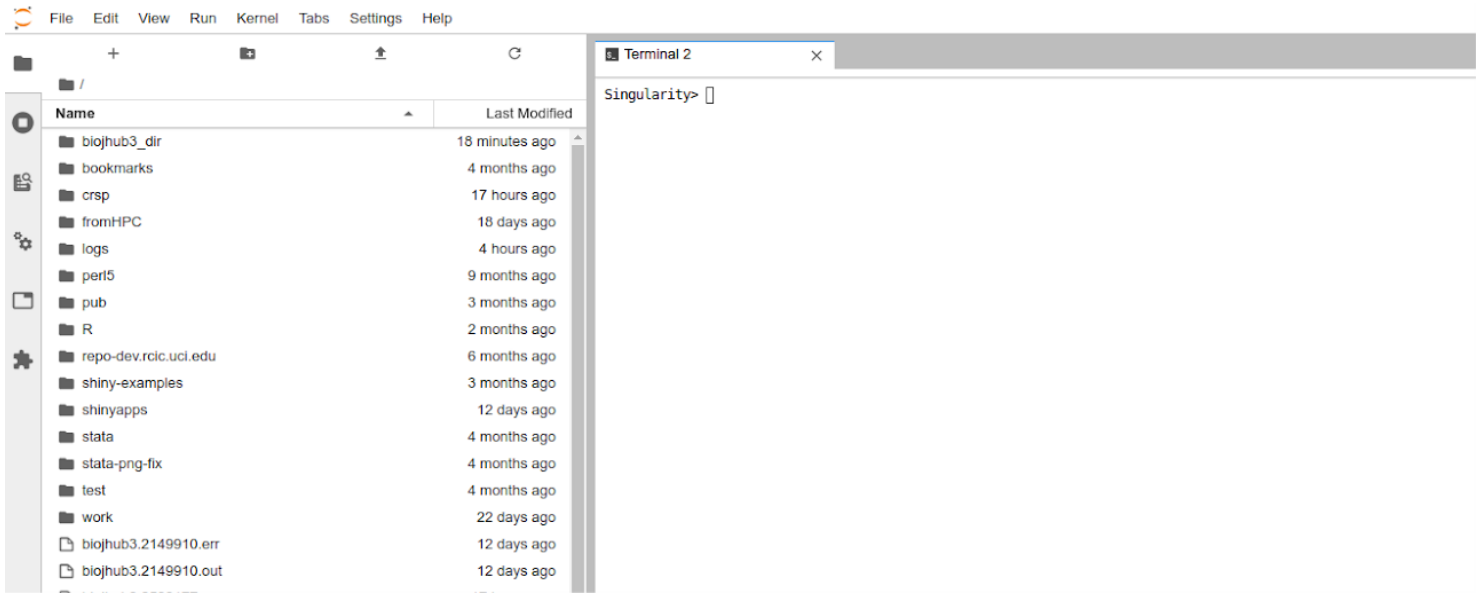


1. File browser GUI
2. Icon quick link
3. File menu -> *Open from Path* will allow you to directly enter the path.

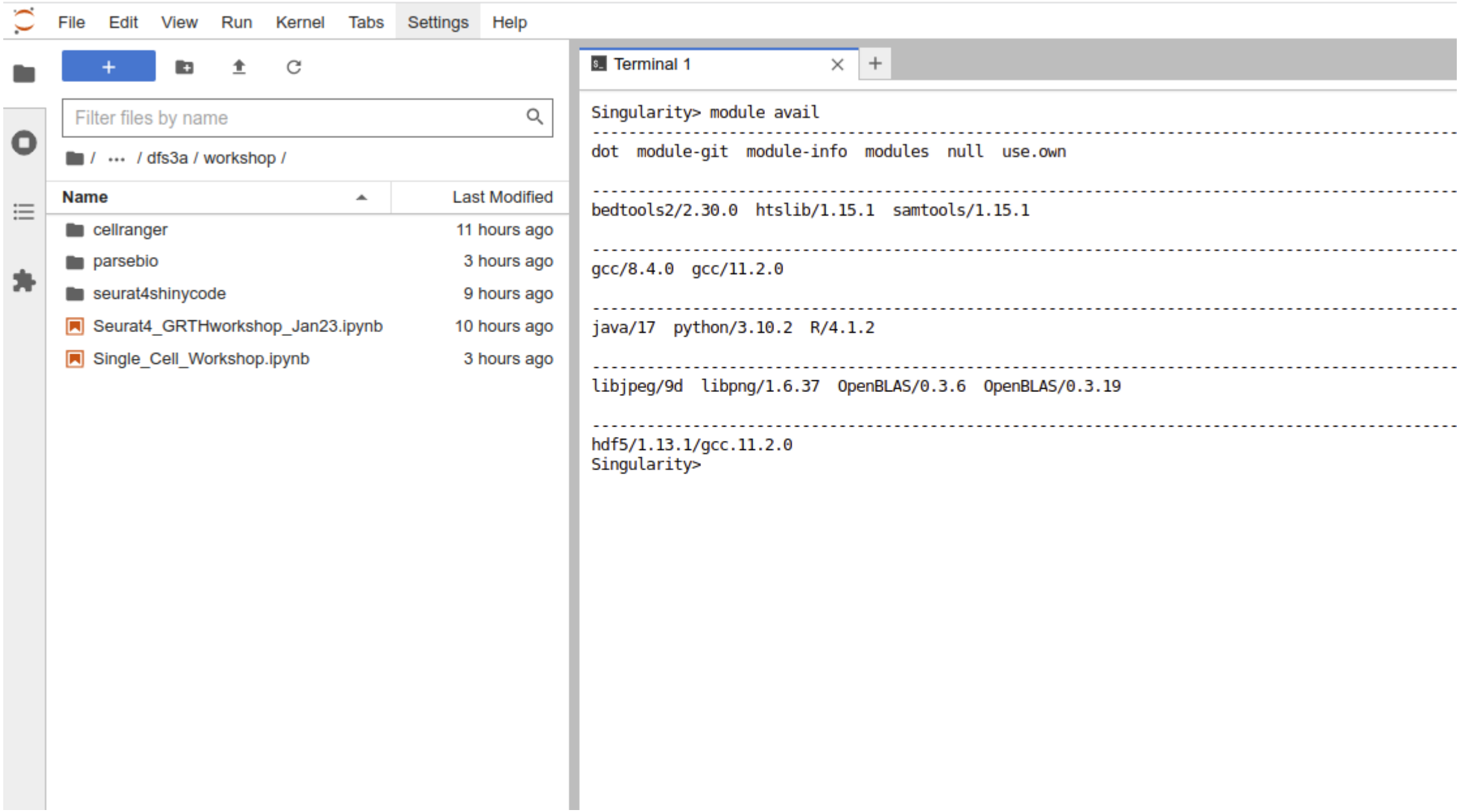
*Due to preventative measures to avoid accidental deposit of files in sensitive areas of HPC3 file system, the root directory of the file browser is set to a fictitious home directory. To quickly traverse to other file systems, several shortcuts are automatically created, serving as symbolic links to the various file systems on HPC3.

Starting a New App (Terminal)

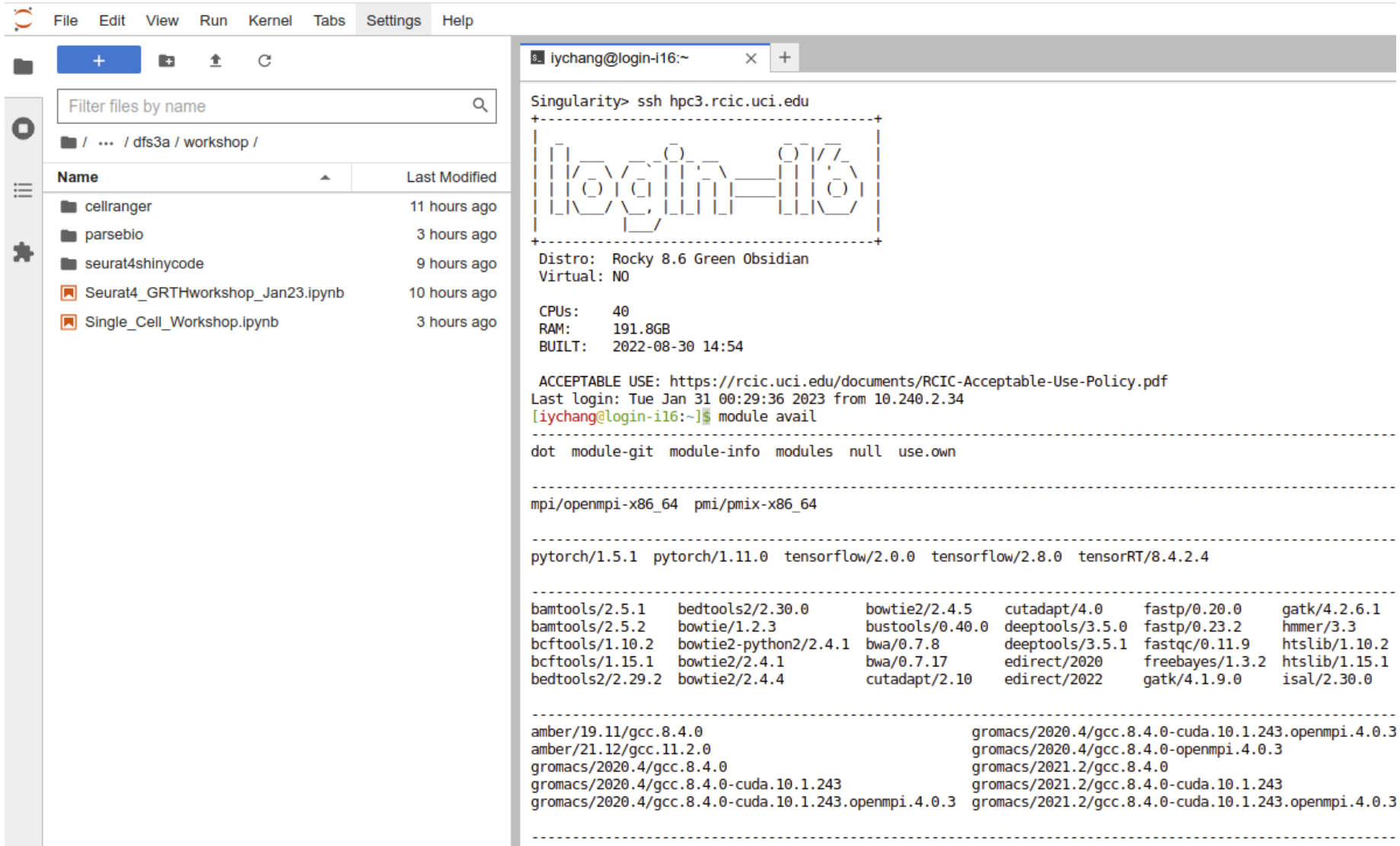




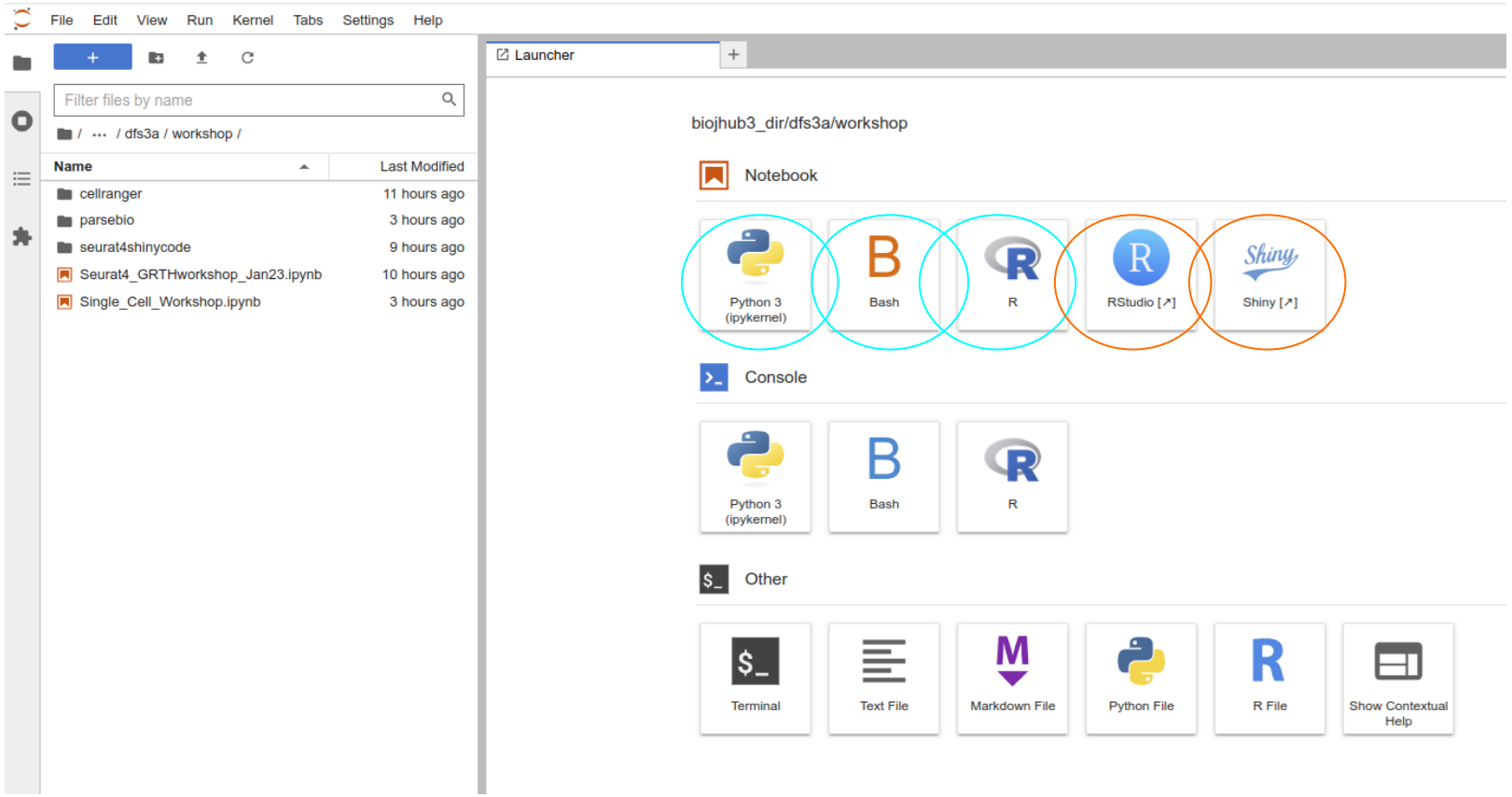
Running Container Modules from Terminal



SSH to HPC3 login node for full software stack



Jupyter Notebook & other web apps

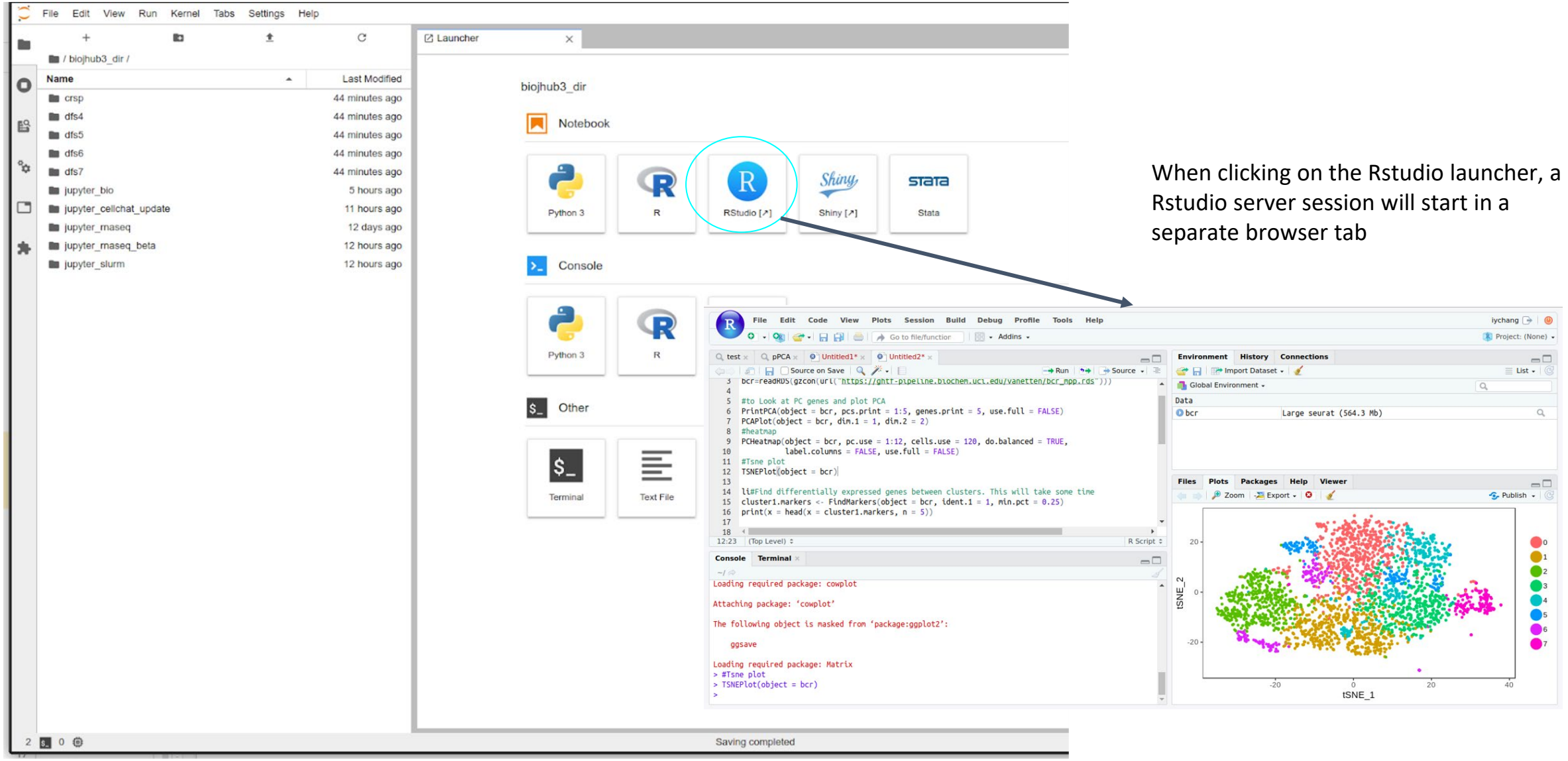


In this container, the user can open either a python, R, or Bash Jupyter computational notebook that will connect to the respective backend kernel and programming language environment.

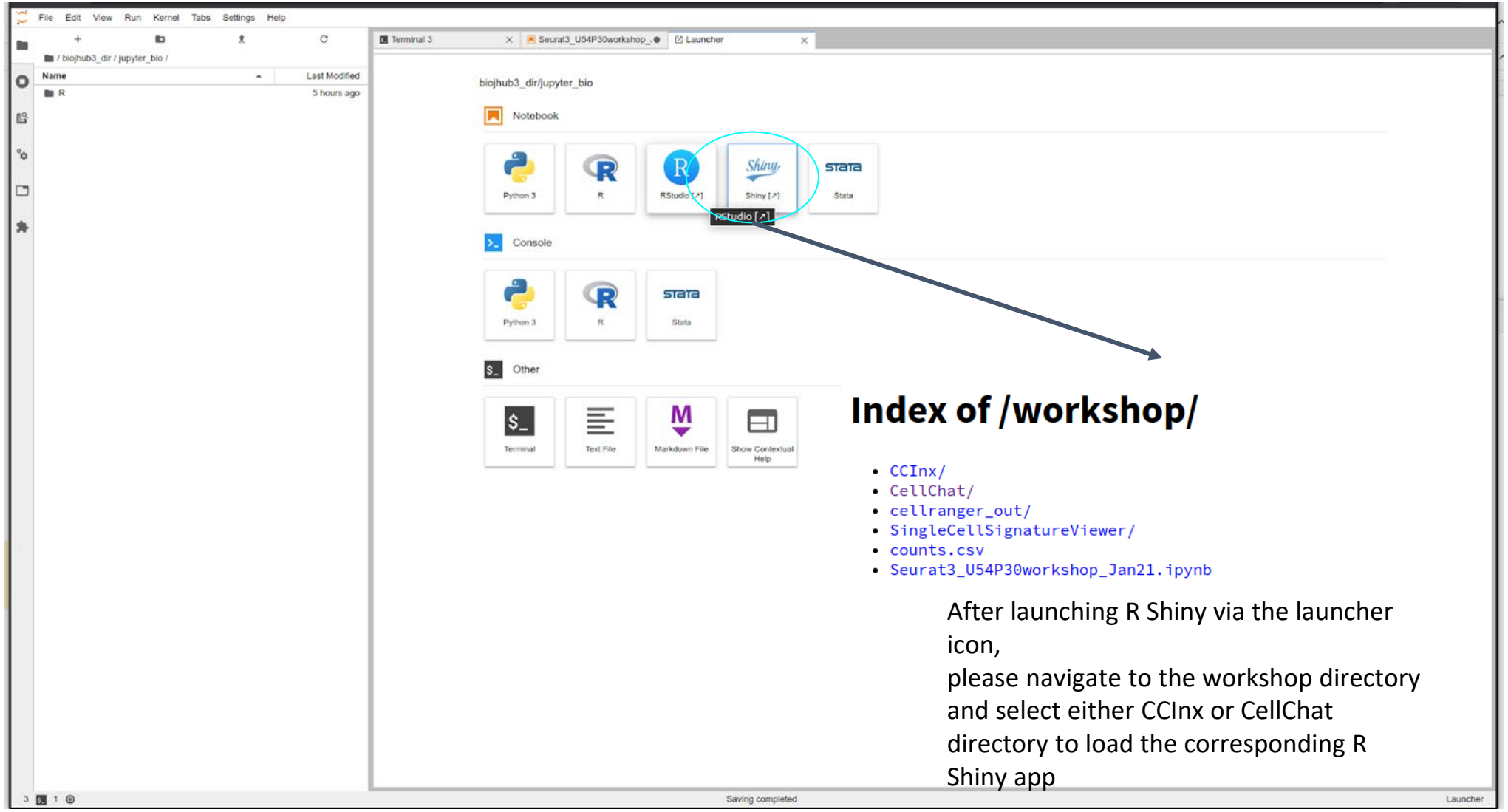
Support for Matlab, Mathematica, and Julia are also available.

In addition, alternative web based development platform such as Rstudio and R Shiny are also available. When you click on these icons, a new browser tab will appear instead of a Jupyter notebook tab.

RStudio


File Edit View Run Kernel Tabs Settings Help
/ biojhub3_dir /
Name
Last Modified
crsp 44 minutes ago
dfs4 44 minutes ago
dfs5 44 minutes ago
dfs6 44 minutes ago
dfs7 44 minutes ago
jupyter_bio 5 hours ago
jupyter_cellchat_update 11 hours ago
jupyter_maseq 12 days ago
jupyter_maseq_beta 12 hours ago
jupyter_slurm 12 hours ago
Launcher
biojhub3_dir
Notebook
Python 3
R
RStudio [↗]
Shiny [↗]
Stata
Console
Python 3
R
Other
Terminal
Text File
Saving completed
When clicking on the Rstudio launcher, a Rstudio server session will start in a separate browser tab
File Edit Code View Plots Session Build Debug Profile Tools Help
iychang
Project: (None)
Environment History Connections
Import Dataset
Global Environment
Data
bcr Large seurat (564.3 Mb)
bcr=readRDS(gzcon(url("https://ghtf-pipeline.biochem.uci.edu/vanetten/bcr_mpp.rds")))
#to Look at PC genes and plot PCA
PrintPCA(object = bcr, pcs.print = 1:5, genes.print = 5, use.full = FALSE)
PCAPlot(object = bcr, dim.1 = 1, dim.2 = 2)
#heatmap
PCHeatmap(object = bcr, pc.use = 1:12, cells.use = 120, do.balanced = TRUE,
label.columns = FALSE, use.full = FALSE)
#Tsne plot
TSNEPlot(object = bcr)
li#Find differentially expressed genes between clusters. This will take some time
cluster1.markers <- FindMarkers(object = bcr, ident.1 = 1, min.pct = 0.25)
print(x = head(x = cluster1.markers, n = 5))
Console Terminal
Loading required package: cowplot
Attaching package: 'cowplot'
The following object is masked from 'package:ggplot2':
ggsave
Loading required package: Matrix
> #Tsne plot
> TSNEPlot(object = bcr)
Files Plots Packages Help Viewer
Zoom Export Publish
tSNE_2
tSNE_1

R Shiny Apps



After launching R Shiny via the launcher icon,
please navigate to the workshop directory and select either CCInx or CellChat directory to load the corresponding R Shiny app

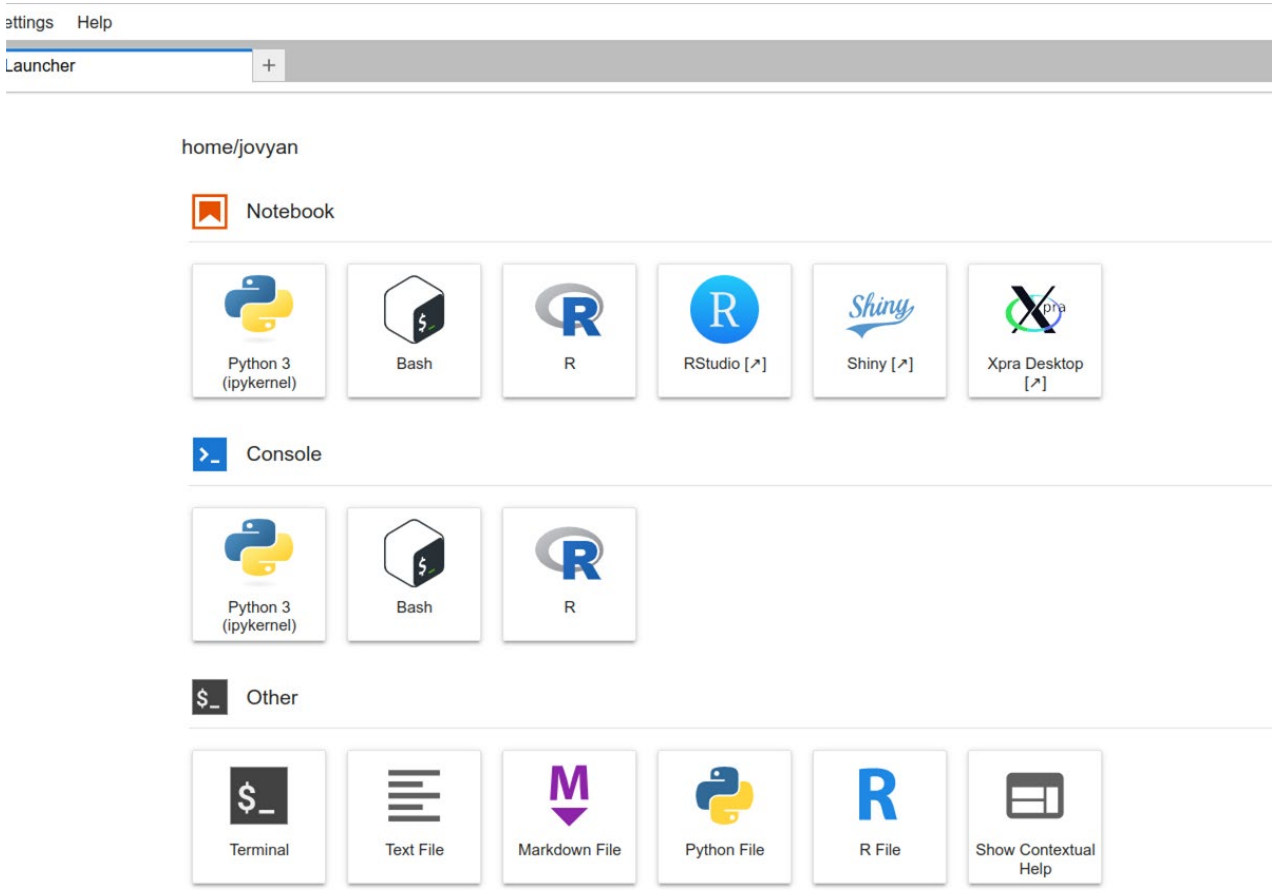
Jupyter Server Proxy

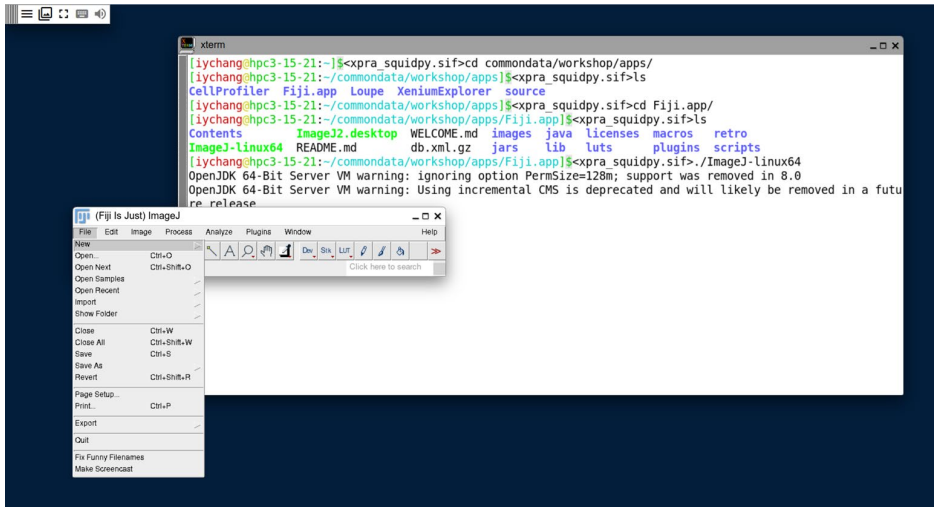
- Allows piggy-backing of other web services through Jupyterhub
- For example:
  - Rstudio server
  - Rshiny Dashboards
  - Xpra X11-to-HTML

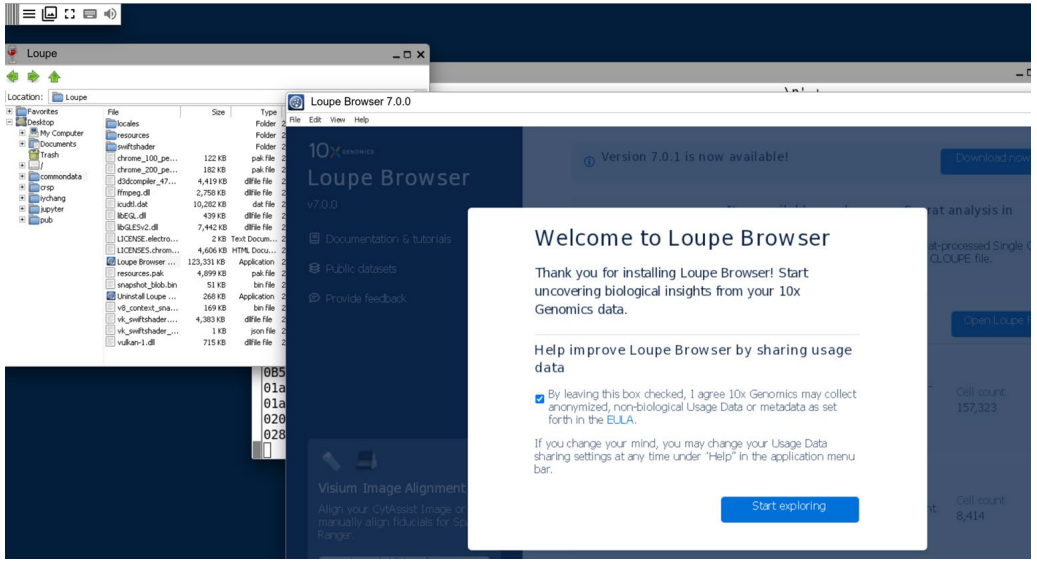
Linux Wine

Enable running windows applications in linux

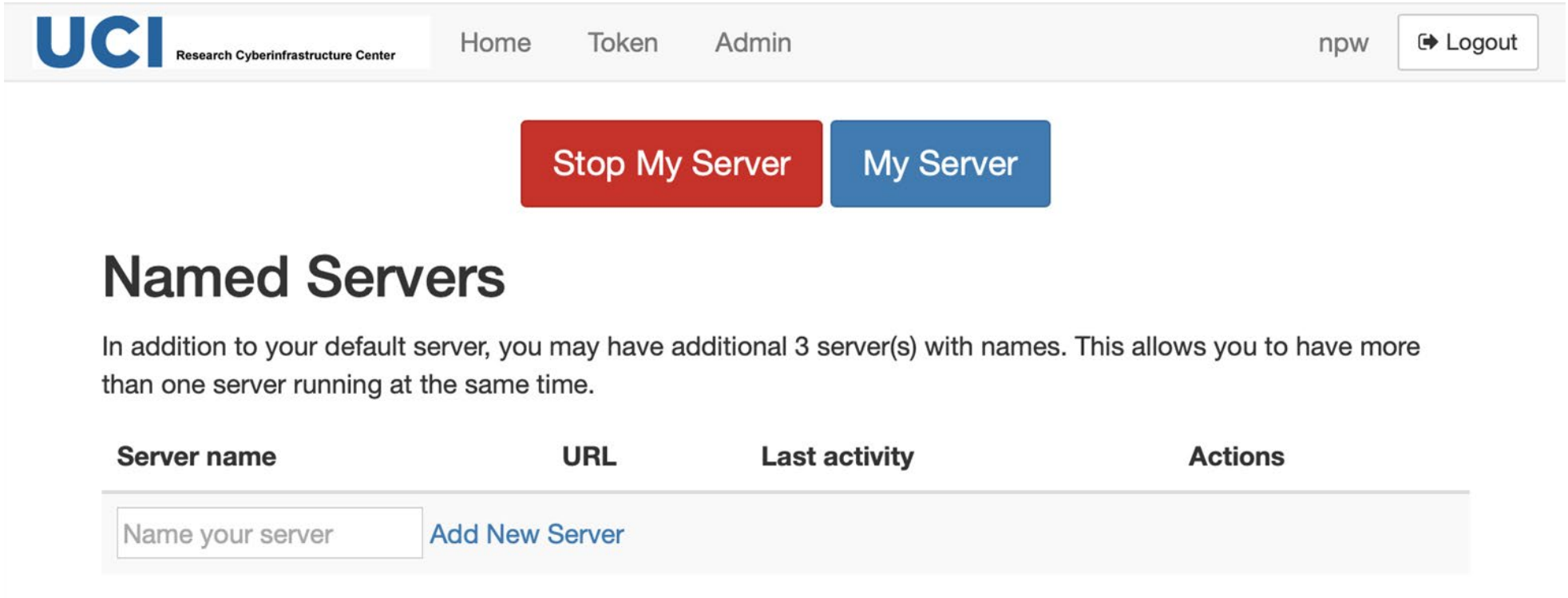
Xpra/Wine via Jupyterhub







Be sure to stop your Juputerhub notebook server after you are done. From the **File** menu choose **Hub Control Panel** and you will be forwarded to a screen similar where you can press on `Stop My Server` to shut down the server:



Spatial-omics Live Demo

- Fiji & CellProfiler
- Loupe Browser & Xenium Explorer
- CellPose & SquidPy

https://hpc3.rcic.uci.edu/biojhub4/

/dfs6/pub/ucightf/workshop/Seurat4_GRTHVisiumworkshop_Sept23.ipynb

/dfs8/commondata/workshop/Seurat4_GRTHVisiumworkshop_Sept23.ipynb

Location of XPRA enabled Spatial-omics Apps

/dfs8/commondata/workshop/apps/CellProfiler
(Windows)

/dfs8/commondata/workshop/apps/Fiji.app
(Linux - X11)

/dfs8/commondata/workshop/apps/Loupe
(Windows)

/dfs8/commondata/workshop/apps/XeniumExplorer
(Windows)

For windows apps, please access via the command: *wine explorer*

XPRA - CellPose Container Specific Instruction

From the xterm in Xpra Desktop, enter:

python -m cellpose

Acknowledgement

GRTHub: Suzanne Sandmeyer, Melanie Oakes, Jenny Wu, Christina Lin

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Joulien Tatar, Nadya Williams