SDSC HPC-DSI 2022:
Interactive Computing

August 2, 2022

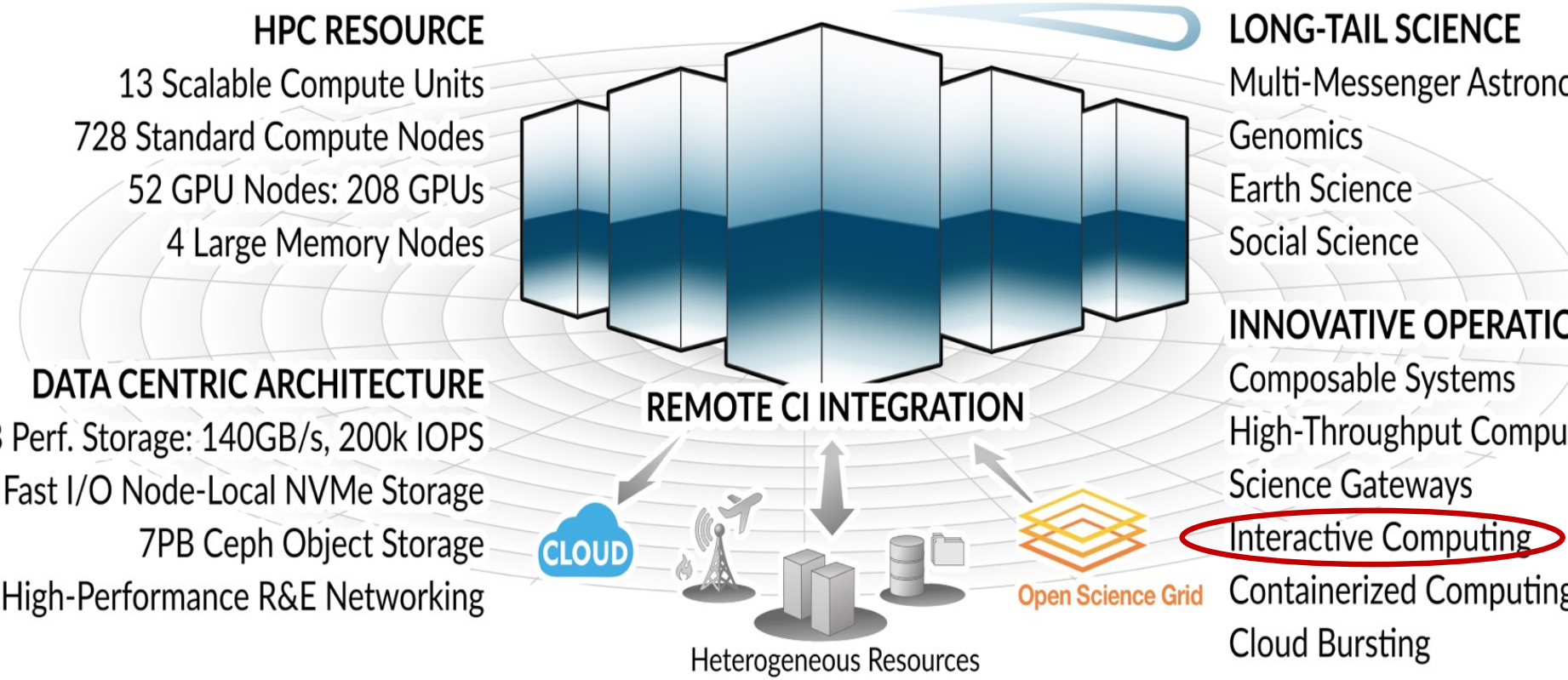
Mary Thomas
SDSC

EXPANSE

COMPUTING WITHOUT BOUNDARIES
5 PETAFLOP/S HPC and DATA RESOURCE

HPC RESOURCE
13 Scalable Compute Units
728 Standard Compute Nodes
52 GPU Nodes: 208 GPUs
4 Large Memory Nodes

DATA CENTRIC ARCHITECTURE
12PB Perf. Storage: 140GB/s, 200k IOPS
Fast I/O Node-Local NVMe Storage
7PB Ceph Object Storage
High-Performance R&E Networking



LONG-TAIL SCIENCE
Multi-Messenger Astronomy
Genomics
Earth Science
Social Science

INNOVATIVE OPERATIONS
Composable Systems
High-Throughput Computing
Science Gateways
Interactive Computing
Containerized Computing
Cloud Bursting

For more details see the Expanse user guide @ https://www.sdsc.edu/support/user_guides/expanse.html
and the "Introduction to Expanse" webinar @ https://www.sdsc.edu/event_items/202006_Introduction_to_Expanse.html

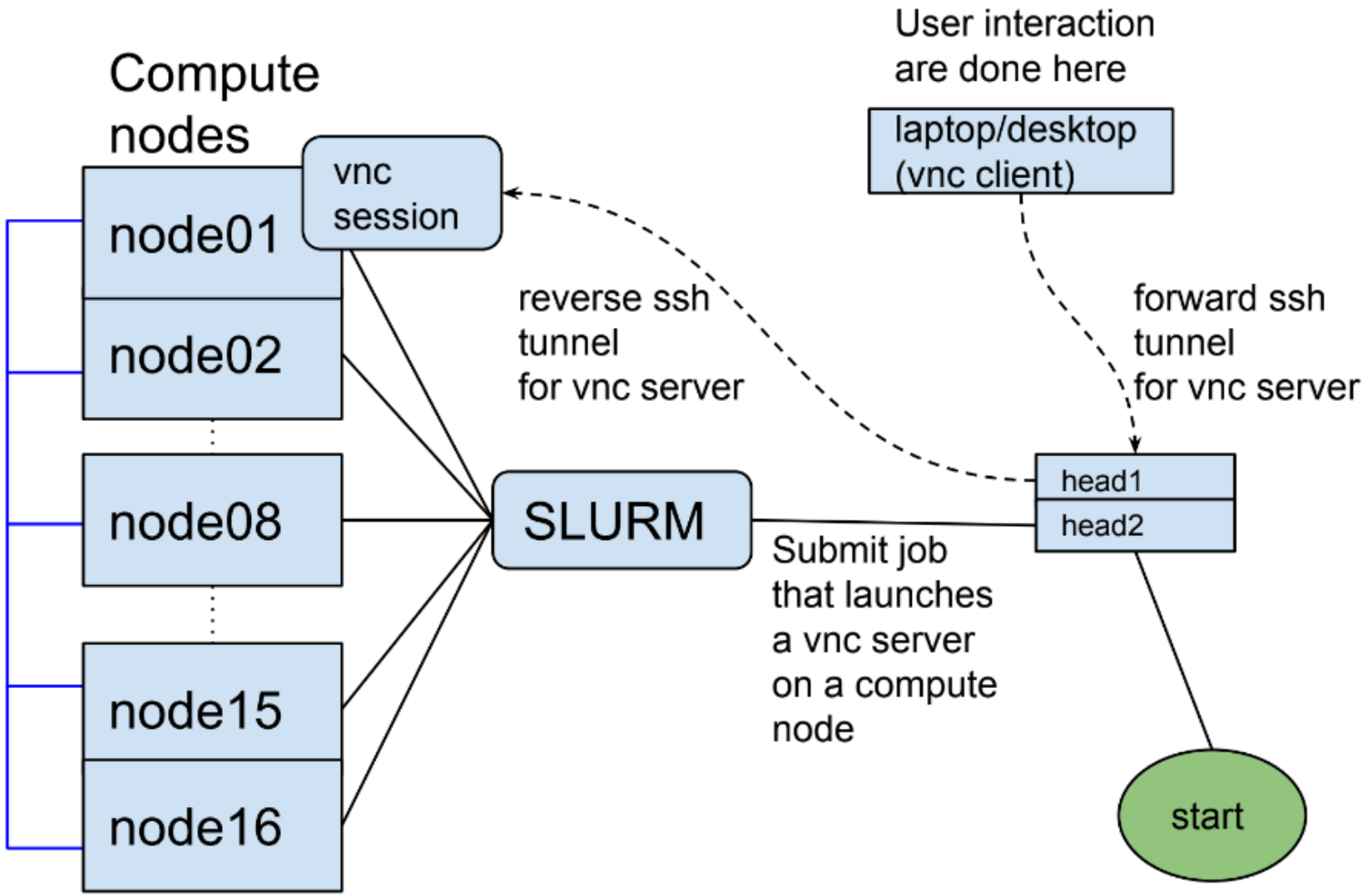
Outline

- What is Interactive High-Performance Computing?
- Accessing Interactive HPC Nodes
- Running Interactive Apps
- Running Interactive Apps Using the Expanse Portal
- Notebook Security

What is Interactive HPC Computing

- In **computer** science, **interactive computing** refers to software which accepts input from the user as it runs.
  - **Interactive** software includes commonly used programs, such as word processors or spreadsheet applications.
- **Interactive HPC computing** involves *real-time* user inputs to perform tasks on a set of compute node(s) including:
  - Code development, real-time data exploration, and visualizations.
  - Used when applications have large data sets or are too large to download to local device, software is difficult install, etc.
  - User inputs come via command line interface or application GUI (Jupyter Notebooks, Matlab, R-studio).
  - Actions performed on remote compute nodes as a result of user input or program out.

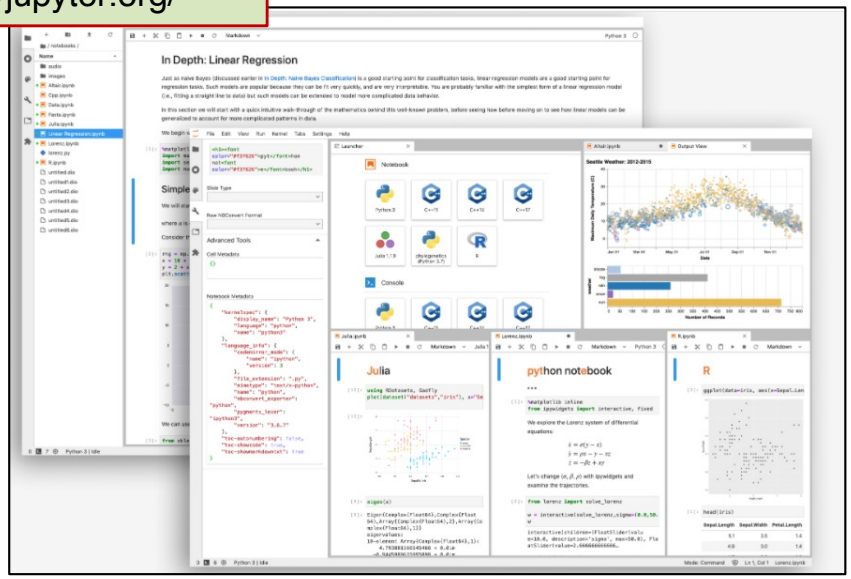
Real-time User Interactions



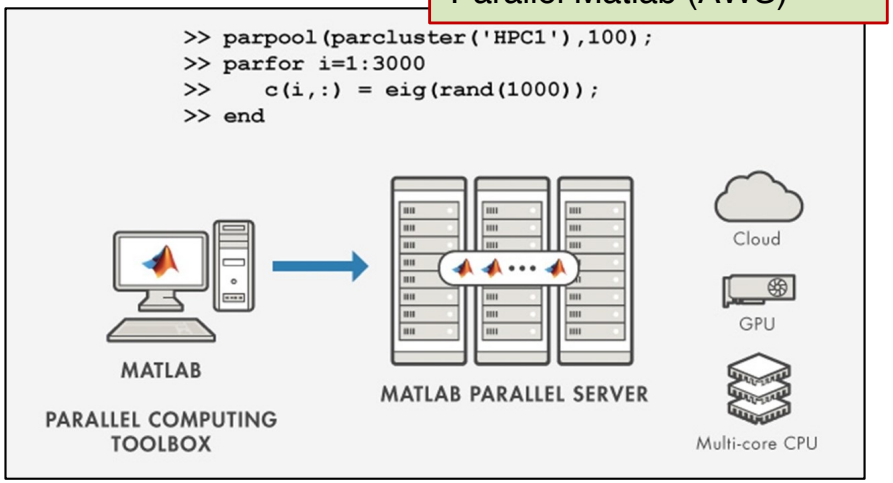
real-time user inputs, perform tasks on a set of compute nodes

Interactive HPC Computing

https://jupyter.org/

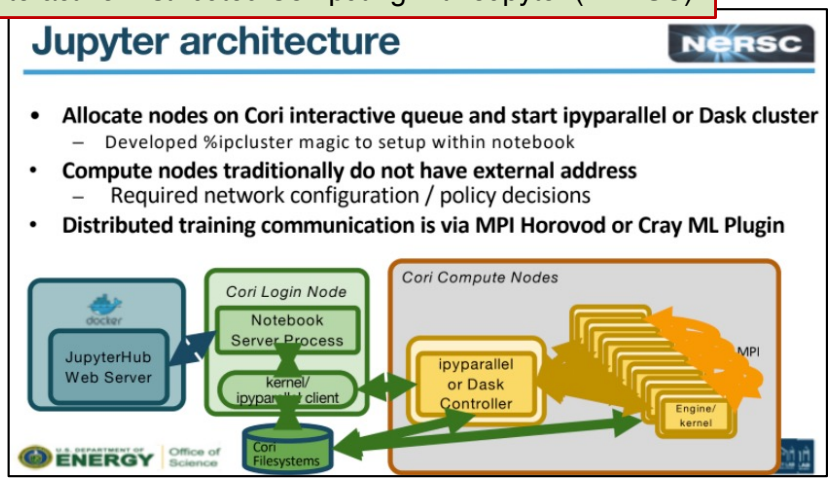


Parallel Matlab (AWS)



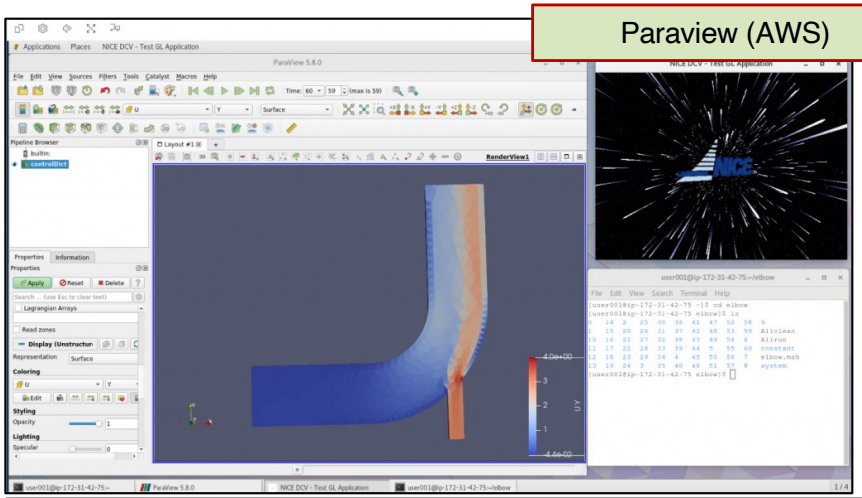
https://azuremarketplace.microsoft.com/en-us/marketplace/apps/mathworks-inc.matlab-parallel-server-listing?tab=Overview

Interactive Distributed Computing with Jupyter (NERSC)



https://drive.google.com/file/d/1-OFjrk1q3L1d3uakr2xkozrPn2c2VZpZ/view

Paraview (AWS)



https://aws.amazon.com/blogs/compute/how-to-run-3d-interactive-applications-with-nice-dcv-in-aws-batch/

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Accessing Interactive Compute Nodes on Expanse

- Connect via terminal using SSH → secure connections
- Use the *srun* command to obtain nodes for 'live,' command line interactive access:

CPU	srun --partition=debug --pty --account=use300 --nodes=1 --ntasks-per-node=4 --mem=8G -t 00:30:00 --wait=0 --export=ALL /bin/bash
GPU	srun --partition=gpu-debug --pty --account=use300 --ntasks-per-node=10 --nodes=1 --mem=96G --gpus=1 -t 00:30:00 --wait=0 --export=ALL /bin/bash

(Tested 7/27/22)

Using An Interactive CPU node

```
[username@login01 openmp]$ module purge
[username@login01 openmp]$ module load slurm
[username@login01 openmp]$ module load cpu
[username@login01 openmp]$ module load gcc/10.2.0
[username@login01 openmp]$ module load openmpi/4.0.4
[username@login01 openmp]$ srun --partition=debug  --pty --account=use300--nodes=1 --ntasks-per-node=64  --mem=128G -t 00:30:00 --wait=0 --export=ALL /bin/bash
```

Request an interactive node for 30 minutes

```
[mthomas@exp-9-55 openmp]$ export OMP_NUM_THREADS=16
[mthomas@exp-9-55 openmp]$ ./hello_openmp
 HELLO FROM THREAD NUMBER =         0
 HELLO FROM THREAD NUMBER =         8
 HELLO FROM THREAD NUMBER =         9
 HELLO FROM THREAD NUMBER =        10
 HELLO FROM THREAD NUMBER =        11
 HELLO FROM THREAD NUMBER =        12
 HELLO FROM THREAD NUMBER =        13
 HELLO FROM THREAD NUMBER =        14
 HELLO FROM THREAD NUMBER =        15
 HELLO FROM THREAD NUMBER =         4
 HELLO FROM THREAD NUMBER =         7
 HELLO FROM THREAD NUMBER =         6
 HELLO FROM THREAD NUMBER =         5
 HELLO FROM THREAD NUMBER =         3
 HELLO FROM THREAD NUMBER =         2
 HELLO FROM THREAD NUMBER =         1
```

- Exit interactive session when your work is done or you will be charged CPU time.
- Beware of oversubscribing your job: don't ask for more cores than you have requested.
- Intel compiler allows this, but your performance will be degraded.

Using An Interactive GPU node

Request an interactive node for 30 minutes

```
[snip]
Last login: Fri Feb 18 12:58:32 2022 from 76.176.117.51
[username @login02 ~]$
[username @login02 ~]$ srun --partition=gpu-shared --pty  --nodes=1  --ntasks-per-node=16 --
mem=374   --gpus=1  -t 00:30:00 --wait=0 --export=ALL --account=use300  /bin/bash
srun: job 9794018 queued and waiting for resources
srun: job 9794018 has been allocated resources
[mthomas@exp-14-57 ~]$
[mthomas@exp-14-57 ~]$ nvidia-smi
Fri Feb 18 13:04:19 2022
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 460.32.03    Driver Version: 460.32.03    CUDA Version: 11.2     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================
|   0  Tesla V100-SXM2...  On   | 00000000:86:00.0 Off |                    0 |
| N/A   34C    P0    41W / 300W |      0MiB / 32510MiB |      0%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================|
|  No running processes found
+-----------------------------------------------------------------------------+
[username @exp-14-57 ~]$ exit
```

Verify you are on a GPU node

Exit when tasks are done

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Viewing Data on HPC Cluster (Simple)

- Cat the file contents
- Plot the data: using gnuplot
- Run Matlab
- Run a data viewing app for the data type:
  - NetCDF, HPF, other

Visualization Apps: Use X11 Forwarding

- On MacOS:
- Install X11 forwarding software:
  - MacOS: Xquartz

```
[mthomas@home]$ brew install --cask xquartz
Updating Homebrew...
Updated 2 taps (homebrew/core and homebrew/cask).
==> New Formulae
[SNIP]
installer: The upgrade was successful.
🍺  xquartz was successfully installed!
quantum:~ mthomas$ which xquartz
/opt/X11/bin/xquartz
```

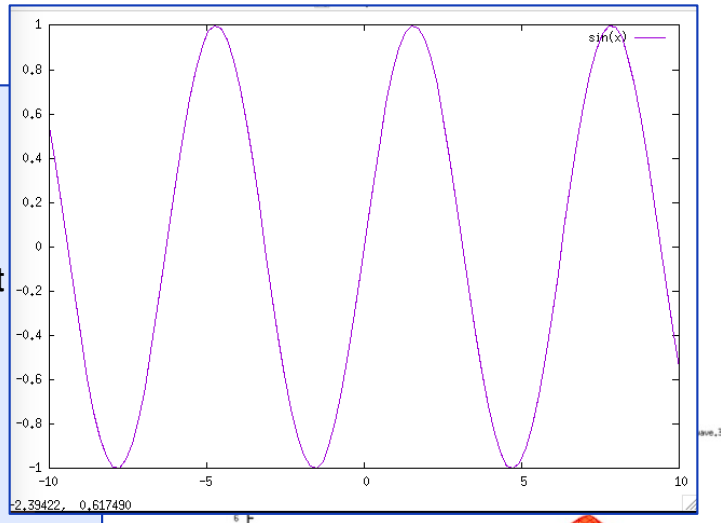
- Use the connection command:

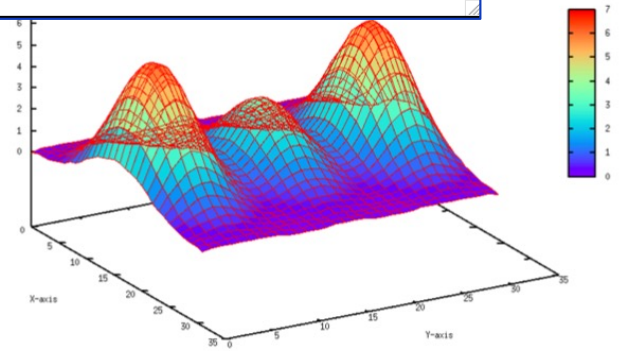
  ssh -Y mthomas@login.expanse.sdsc.edu'

gnuplot

- *gnuplot* is a command-driven interactive function plotting program. It can be used to plot functions and data points in both two- and three- dimensional plots in many different formats.
- It is designed primarily for the visual display of scientific data.
- Can be run from the gnuplot app or from within your program so you can save visualizations of results.

```
module load cpu/0.15.4 gcc/10.2.0
[mthomas@login01 ~]$ module load gnuplot/5.2.8
[mthomas@login01 ~]$ which gnuplot
/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen2/gcc-
10.2.0/gnuplot-5.2.8-uwugzxg4dgxaiciheiepgol67cw7m6yg/bin/gnuplot
[mthomas@login01 gnuplot-ex]$ gnuplot
G N U P L O T
Version 5.2 patchlevel 8    last modified 2019-12-01
Copyright (C) 1986-1993, 1998, 2004, 2007-2019
Thomas Williams, Colin Kelley and many others
gnuplot home:     http://www.gnuplot.info
faq, bugs, etc:   type "help FAQ"
immediate help:   type "help"  (plot window: hit 'h')
Terminal type is now 'x11'
gnuplot> plot sin(x)
gnuplot>
```





https://alvinalexander.com/technology/gnuplot-charts-graphs-examples/

Expanse: Matlab from the command line

```
[mthomas@login01 ~]$ srun --partition=debug  --pty --account=use300 --nodes=1 --ntasks-per-
node=4  --mem=8G -t 00:30:00 --wait=0 --export=ALL /bin/bash
srun: job 14833549 queued and waiting for resources
srun: job 14833549 has been allocated resources
[mthomas@exp-9-55 ~]$ module list
Currently Loaded Modules:
  1) shared   2) slurm/expanse/21.08.8   3) sdsc/1.0   4) DefaultModules   5) cpu/0.15.4   6)
gcc/10.2.0   7) gnuplot/5.2.8

[mthomas@exp-9-55 ~]$ module list
Currently Loaded Modules:
  1) shared   2) slurm/expanse/21.08.8   3) sdsc/1.0   4) DefaultModules   5) cpu/0.15.4   6)
gcc/10.2.0   7) gnuplot/5.2.8
[mthomas@exp-9-55 ~]$ module load matlab/2022a
[mthomas@exp-9-55 ~]$ matlab
MATLAB is selecting SOFTWARE OPENGL
rendering.                                                    < M A T L A B (R)>
  Copyright 1984-2022 The MathWorks, Inc.
      R2022a (9.12.0.1884302) 64-bit (glnxa64)
                      February 16, 2022
 >> a = [1 3 5; 2 4 6; 7 8 10]
a =
   1   3   5
   2   4   6
   7   8  10
>> b=sin(a)
b =
  0.8415   0.1411  -0.9589
  0.9093  -0.7568  -0.2794
  0.6570   0.9894  -0.5440
>> plot(b)
>>
```

UCSD Triton Shared Computing Cluster (TSCC)
Interactive Job: Hello-MPI

qsub –I -l nodes=2:ppn=10 -l walltime=0:50:00

```
[mthomas@tscc-gpu-9-4 hello-mpi]$
[mthomas@tscc-gpu-9-4 hello-mpi]$ qsub -I -l nodes=1:ppn=16 -l walltime=0:30:00 -q glean
qsub: waiting for job 26842841.tscc-mgr7.local to start
qsub: job 26842841.tscc-mgr7.local ready

[mthomas@tscc-gpu-9-4 ~]$ pwd
[mthomas@tscc-gpu-9-4 hello-mpi]$ mpirun -np 8 ./hello-mpi
 node        0 : Hello and Welcome to TSCC!
 node        6 : Hello and Welcome to TSCC!
 node        1 : Hello and Welcome to TSCC!
 node        3 : Hello and Welcome to TSCC!
 node        4 : Hello and Welcome to TSCC!
 node        5 : Hello and Welcome to TSCC!
 node        7 : Hello and Welcome to TSCC!
 node        2 : Hello and Welcome to TSCC!
```

Request interactive node using glean queue node

Interactive nodes can be used for running parallel jobs (MPI, OpenMP, CUDA code if GPU), compiling large codes, viz apps.

TSCC Interactive Jobs: Applications Running Matlab without GUI

qsub –I –l nodes=1:ppn=16 walltime=0:30:00 –q glean

```
[mthomas@tscc-login1 hello-mpi]$ qsub -I -l nodes=1:ppn=16 -l
walltime=0:30:00 -q glean
qsub: waiting for job 26842936.tscc-mgr7.local to start
qsub: job 26842936.tscc-mgr7.local ready


[mthomas@tscc-13-12 ~]$ module load matlab
[mthomas@tscc-13-12 ~]$ matlab -nodisplay
               < M A T L A B (R) >
      Copyright 1984-2016 The MathWorks, Inc.
      R2016b (9.1.0.441655) 64-bit (glnxa64)
                September 7, 2016

To get started, type one of these: helpwin, helpdesk, or demo.
For product information, visit www.mathworks.com.
```

```
>>  A = [1 3 0; 2 4 -1; 4 9 -1]
A =
     1     3     0
     2     4    -1
     4     9    -1
>> B=A'
B =
     1     2     4
     3     4     9
     0    -1    -1
>> A*B
ans =
    10    14    31
    14    21    45
    31    45    98
>> exit
[mthomas@tscc-13-12 ~]$
```

TSCC Interactive Jobs: Launching Matlab with GUI

To use a Graphical User Interface (GUI) as part of your interactive job, you will need to set up Xforwarding. Example below is for using XQuartz on a MAC. For examples for MacOS and Windows, see: http://systems.eecs.tufts.edu/x11-forwarding/

Step 1: *Set X11 forwarding on the computer that you are connecting from: Update or install Xquartz and* ***restart*** *your system*

```
[mthomas@home]$ brew install --cask xquartz
Updating Homebrew...
Updated 2 taps (homebrew/core and homebrew/cask).
==> New Formulae
[SNIP]
installer: The upgrade was successful.
🍺  xquartz was successfully installed!
quantum:~ mthomas$ which xquartz
/opt/X11/bin/xquartz
```

Step 2: *Log on to TSCC, using* ***–Y*** *option (trusted)*

```
[mthomas@home]$ ssh -Y tscc-login.sdsc.edu -lmthomas
```

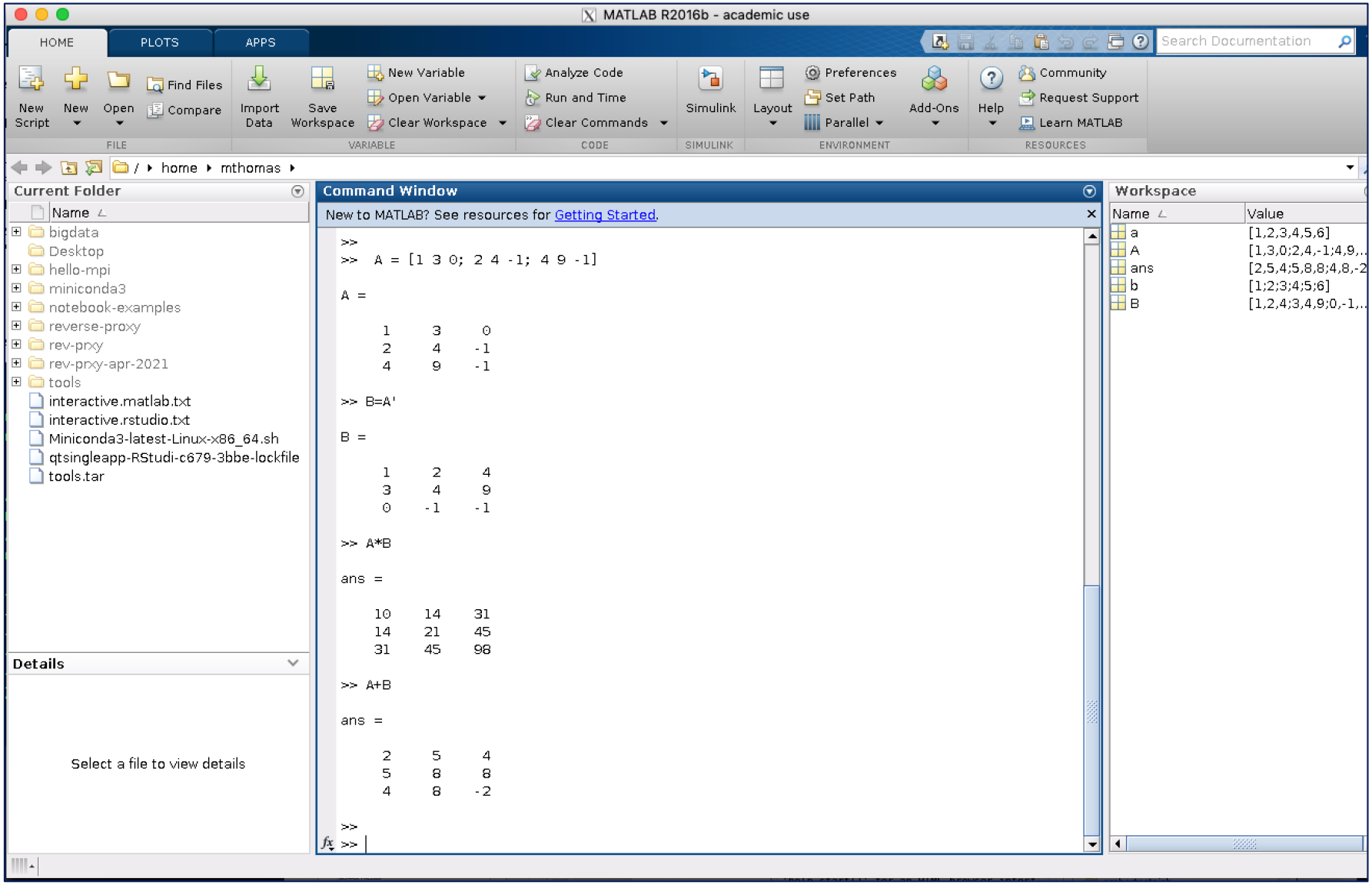
Step 3: *Request an interactive node, using* ***–X*** *option*

```
[mthomas@tscc-login1 hello-mpi]$ qsub -I -X -l
nodes=1:ppn=1 -q glean
qsub: waiting for job 26843028.tscc-mgr7.local to start
qsub: job 26843028.tscc-mgr7.local ready
[mthomas@tscc-4-46 ~]$
```

Step 4: *Setup your module environment and run Matlab*

```
[mthomas@tscc-4-46 ~]$ module load matlab
[mthomas@tscc-4-46 ~]$ matlab
MATLAB is selecting SOFTWARE OPENGL rendering.
```

TSCC Interactive Jobs: Running Matlab with GUI



TSCC Interactive Jobs: Running R console (no GUI)

Step 3: *Request an interactive node, using* ***–X*** *option*

```
[mthomas@tscc-login2 ~]$ qsub -I -q glean -l nodes=1:ppn=1
qsub: waiting for job 26844488.tscc-mgr7.local to start
qsub: job 26844488.tscc-mgr7.local ready
[mthomas@tscc-4-46 ~]$
```

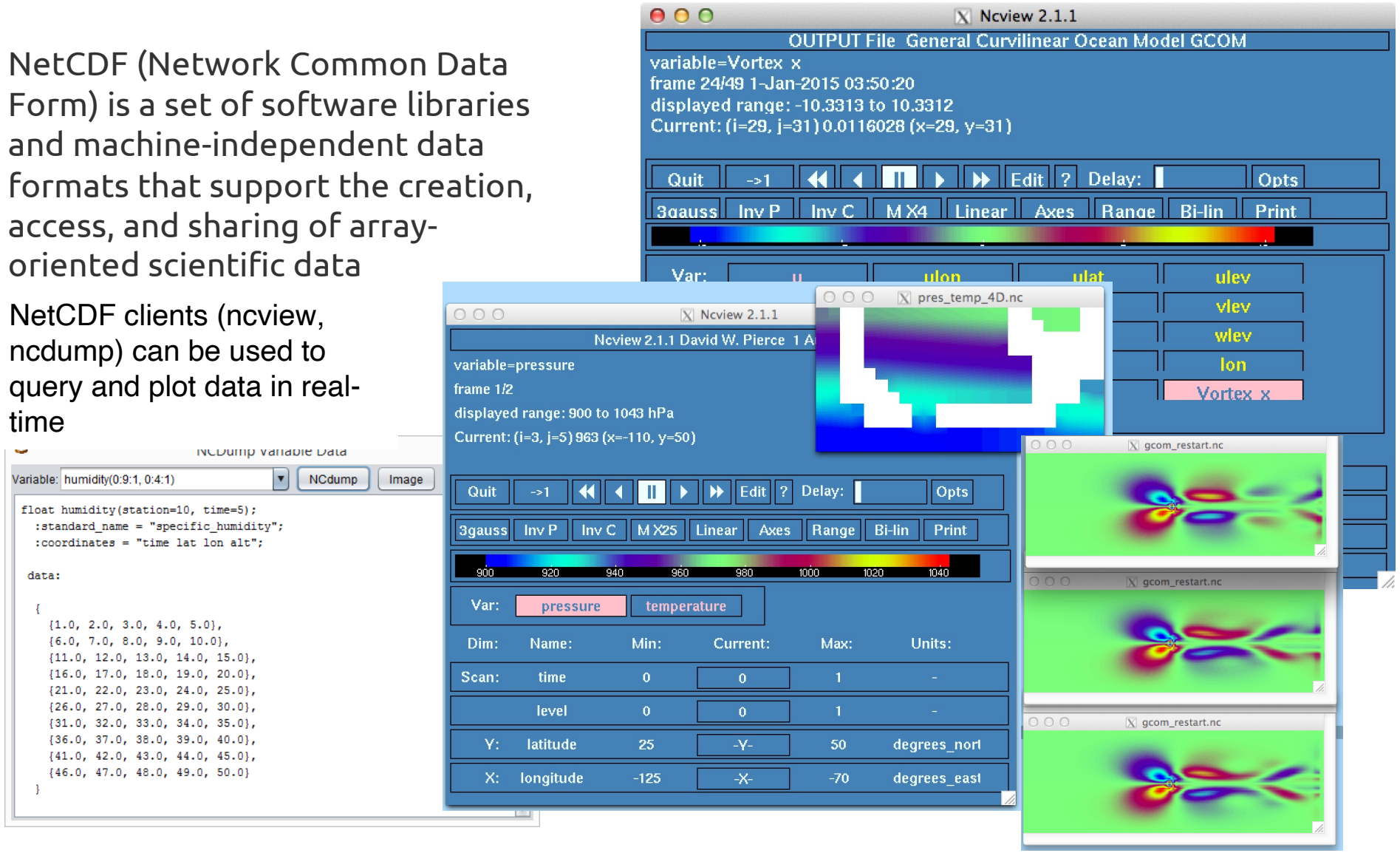
Step 4: *Setup your module environment and run Matlab*

```
[mthomas@tscc-4-46 ~]$ module load R
Unloading compiler-dependent module openmpi_ib/3.1.4
[mthomas@tscc-4-46 ~]$ R
R version 4.0.2 (2020-06-22) -- "Taking Off Again"
Copyright (C) 2020 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)

R is free software and comes with ABSOLUTELY NO WARRANTY.
[SNIP]
R is a collaborative project with many contributors.
[SNIP]
> myString <- "Hello, World!"
> print ( myString )
[1] "Hello, World!"
>
```

Viewing NetCDF Files

- NetCDF (Network Common Data Form) is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data
- NetCDF clients (ncview, ncdump) can be used to query and plot data in real-time



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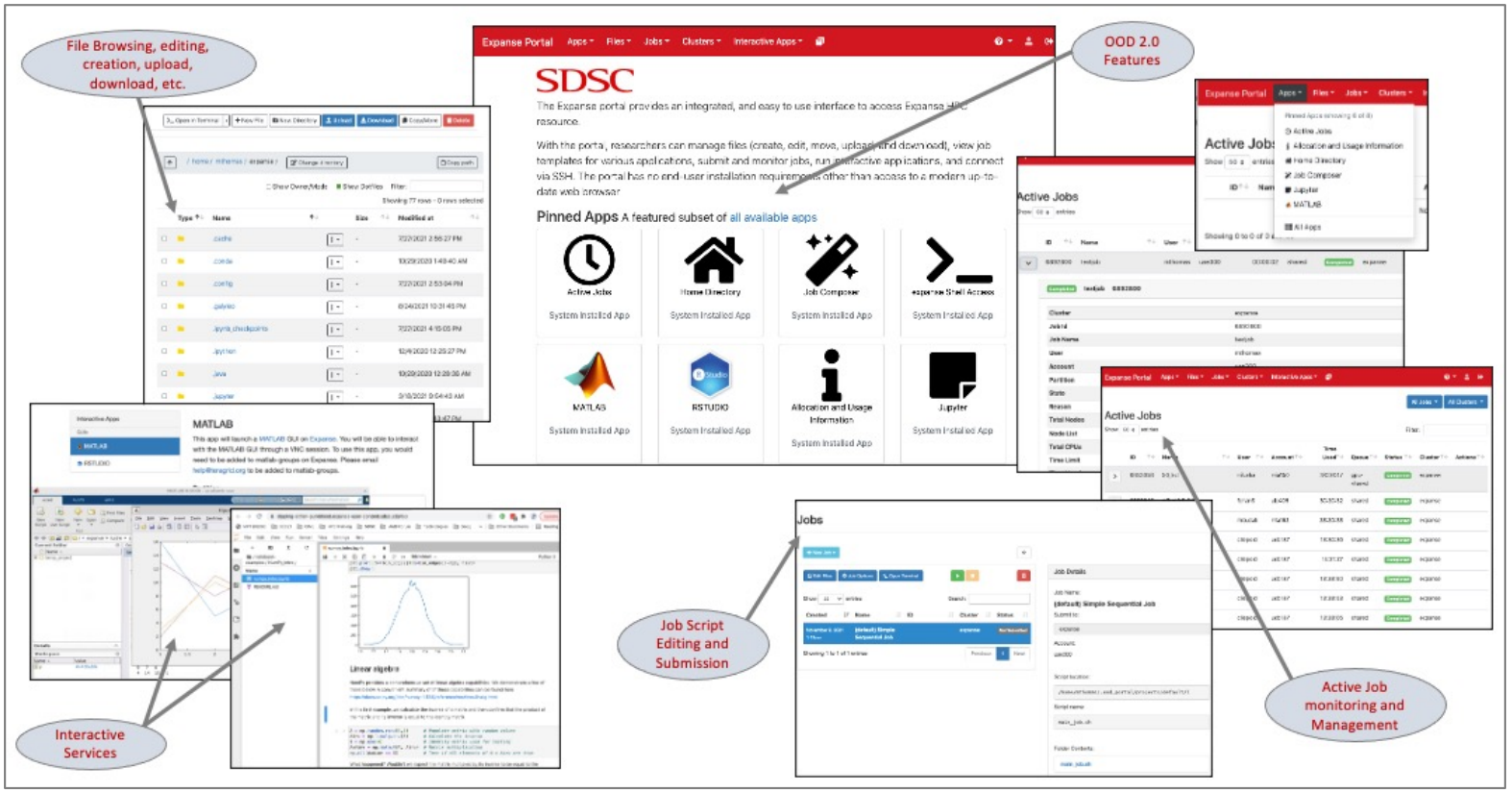
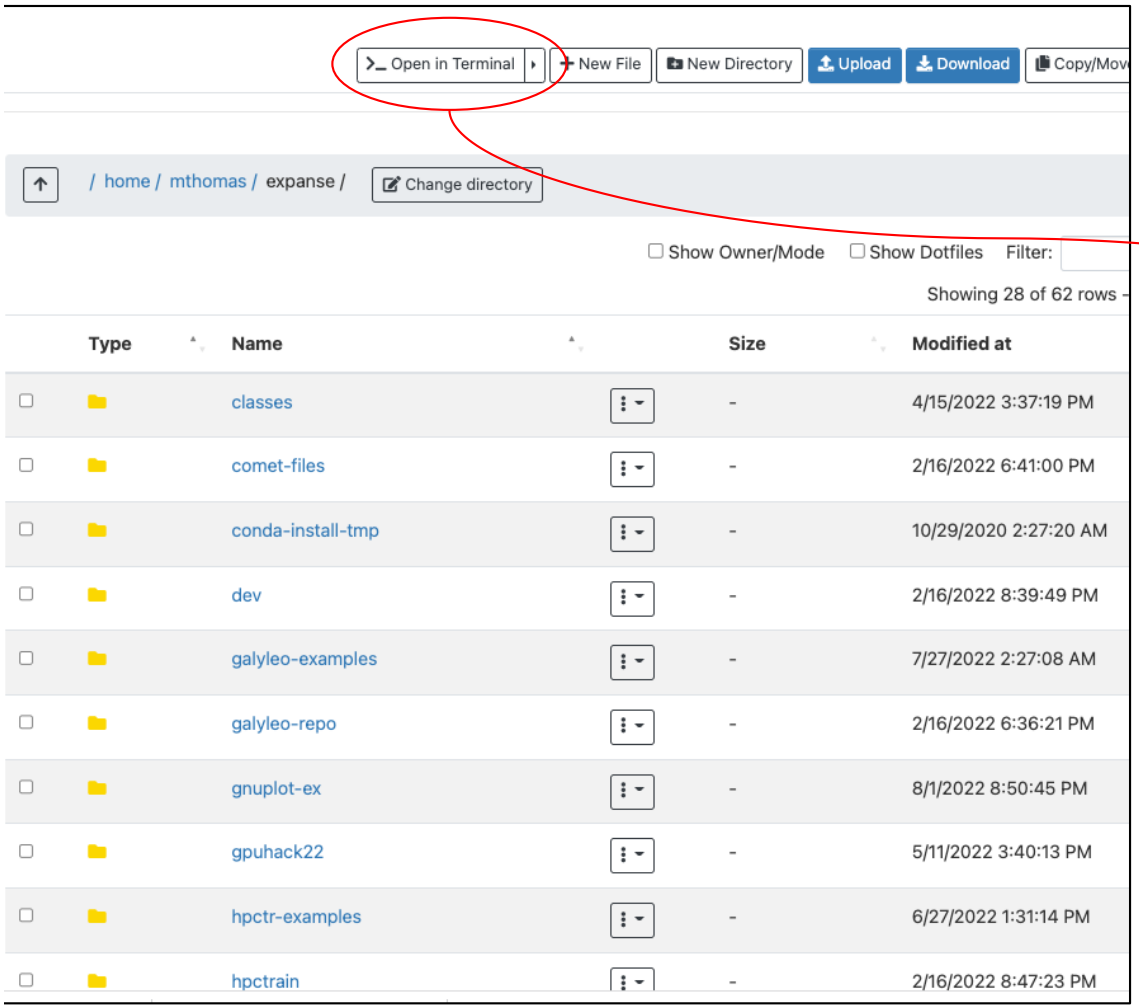
Expanse User Portal

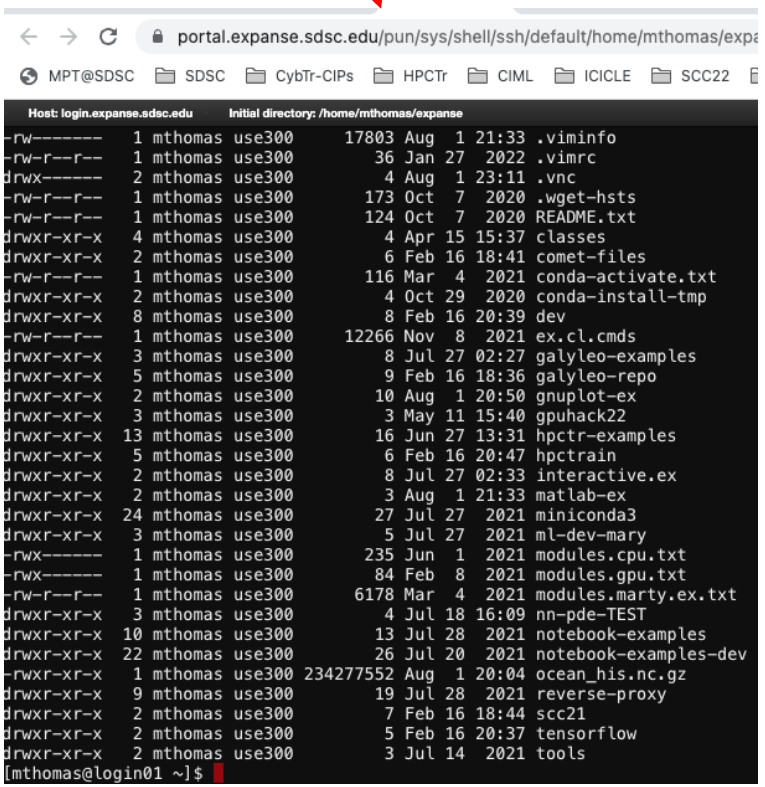


- https://portal.expanse.sdsc.edu; access using XSEDE credentials
- Securely hosts batch job submission & monitoring, and interactive applications
- Portal simplifies launching supported interactive applications → manages software dependencies

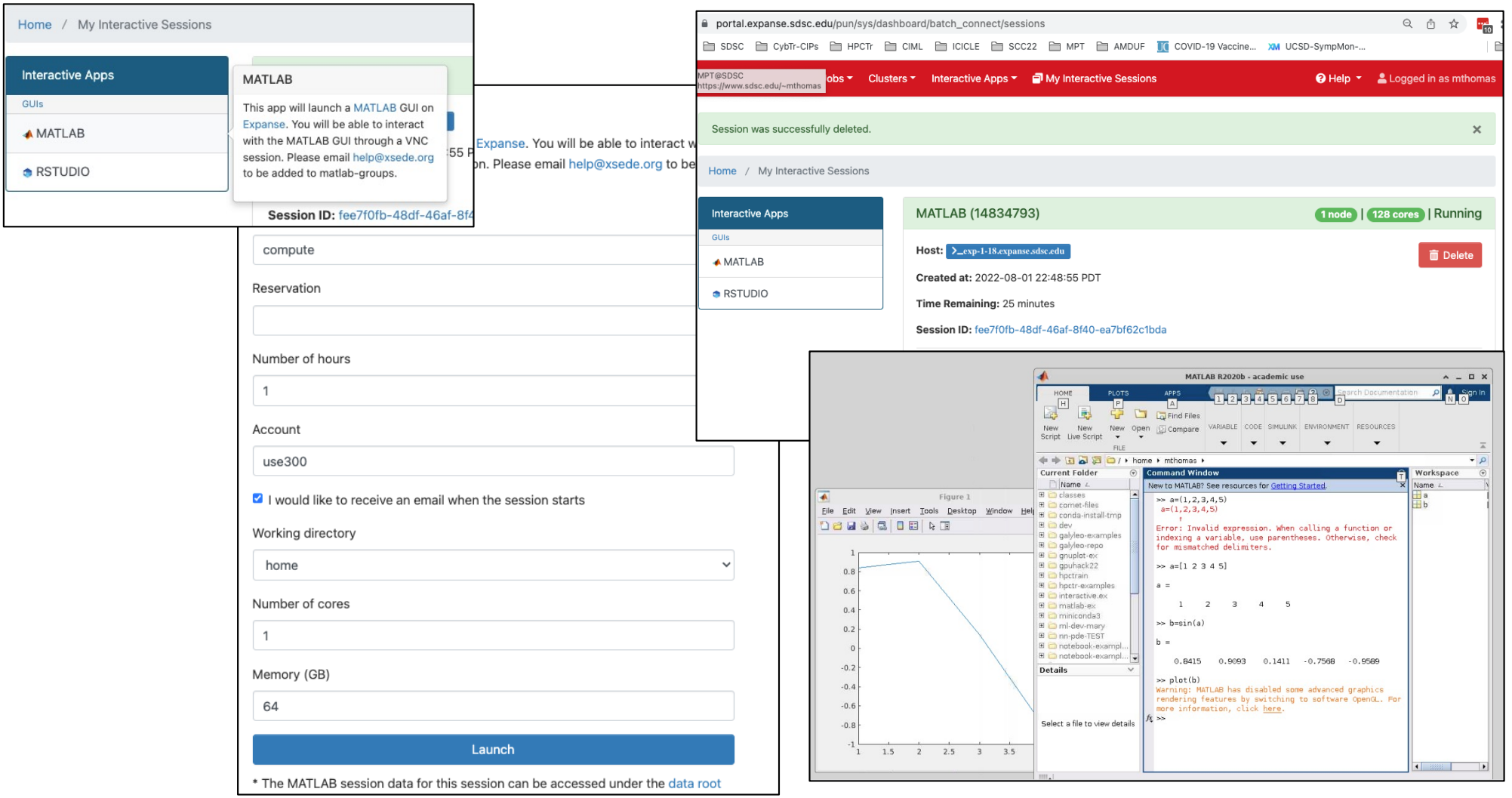
Sivagnanam, S., Irving, C., Kandes, M., Mishin, D., Sakai, S., Strande, S., Tatineni, M., Thomas, M., Norman, M. (2021). Experiences in building a user portal for Expanse supercomputer. *PEARC21: Practice and Experience in Advanced Research Computing*, Accepted. ACM. https://doi.org/10.1145/3437359.3465590

Expanse Portal: File Management

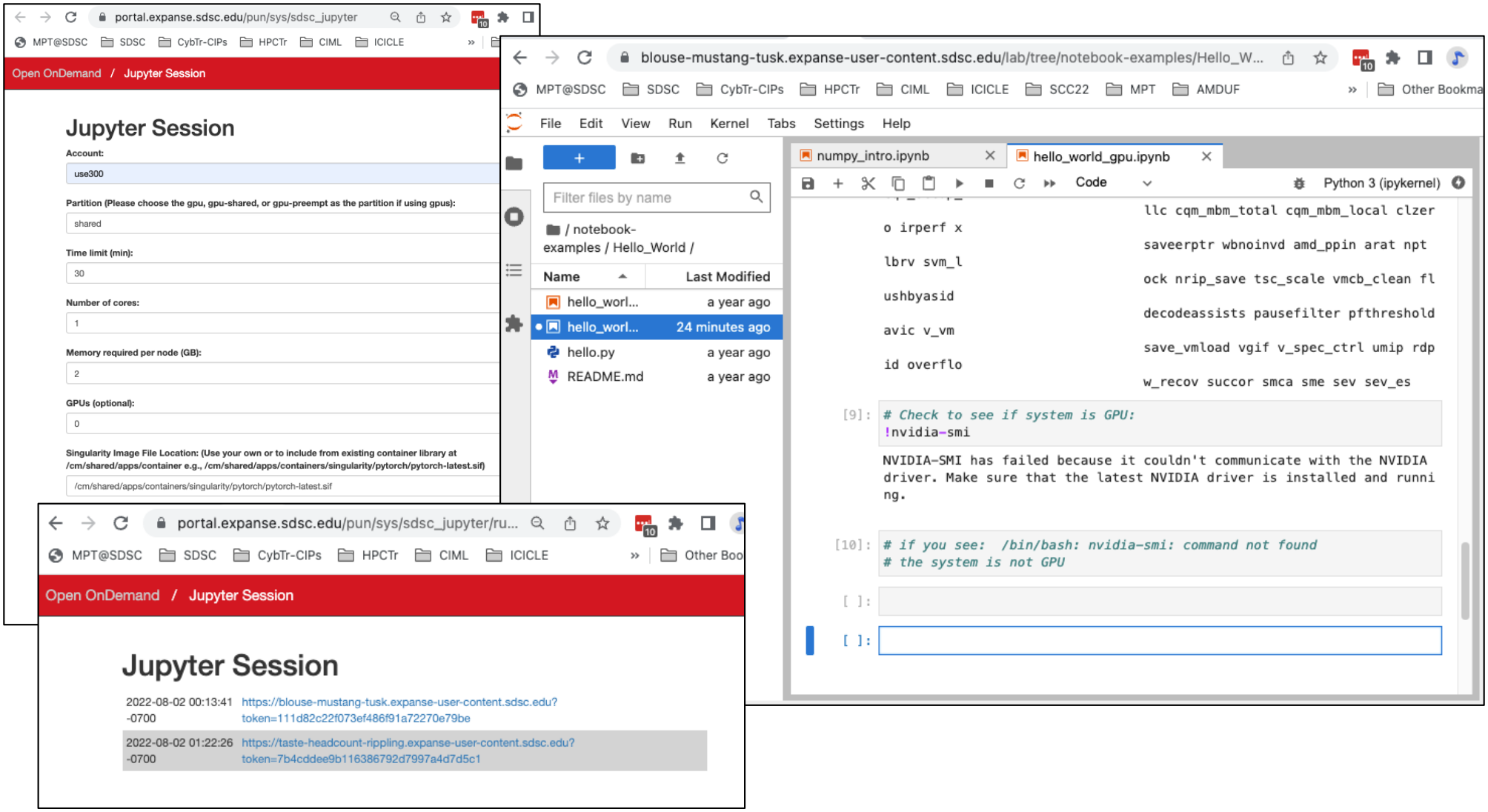




Expanse Portal: Running Matlab



Expanse Portal: Launching Notebooks



- PORTAL LIVE DEMO

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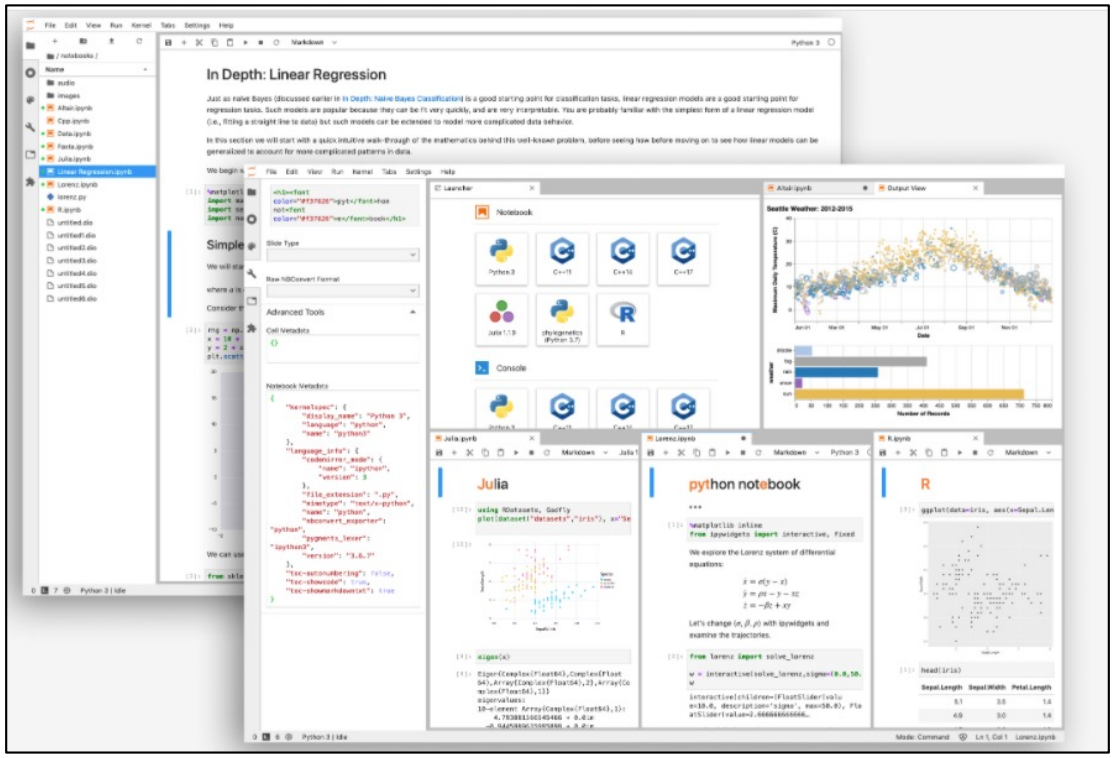
Juptyer Notebooks

What is Jupyter?

Jupyter *is a free, open-source, interactive web tool known as a computational notebook, which researchers can use to combine software code, computational output, explanatory text and multimedia resources in a single document.* *(J. Perkel, https://www.nature.com/articles/d41586-018-07196-1)*

Common Jupyter Services:

- Jupyter Notebooks (single user)
- JupyterLab: advanced version of notebook
- JupyterHub: multiuser Jupyter service



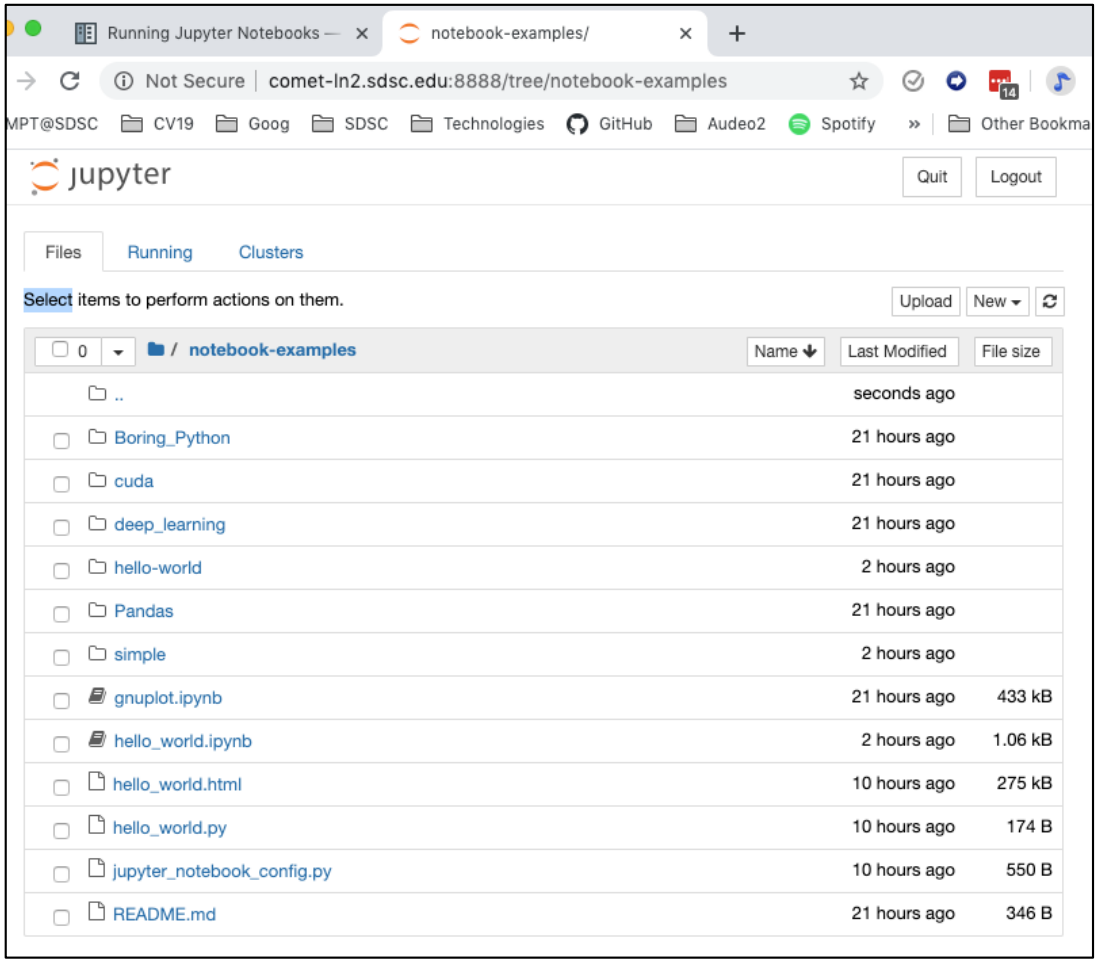
Interactive Services have a Key Vulnerability: They Provide Access to HPC File Systems, often over HTTP

SDSC Interactive Services Policy:

- Portals, JupyterHub, and other services cannot be mounted directly to disk (must be on VM or external)
  - Many use root in vulnerable ways
  - If a user launches Jupyter Lab or Notebooks, the jobs will be killed.
- Applications cannot run on login nodes

SDSC recommendation:

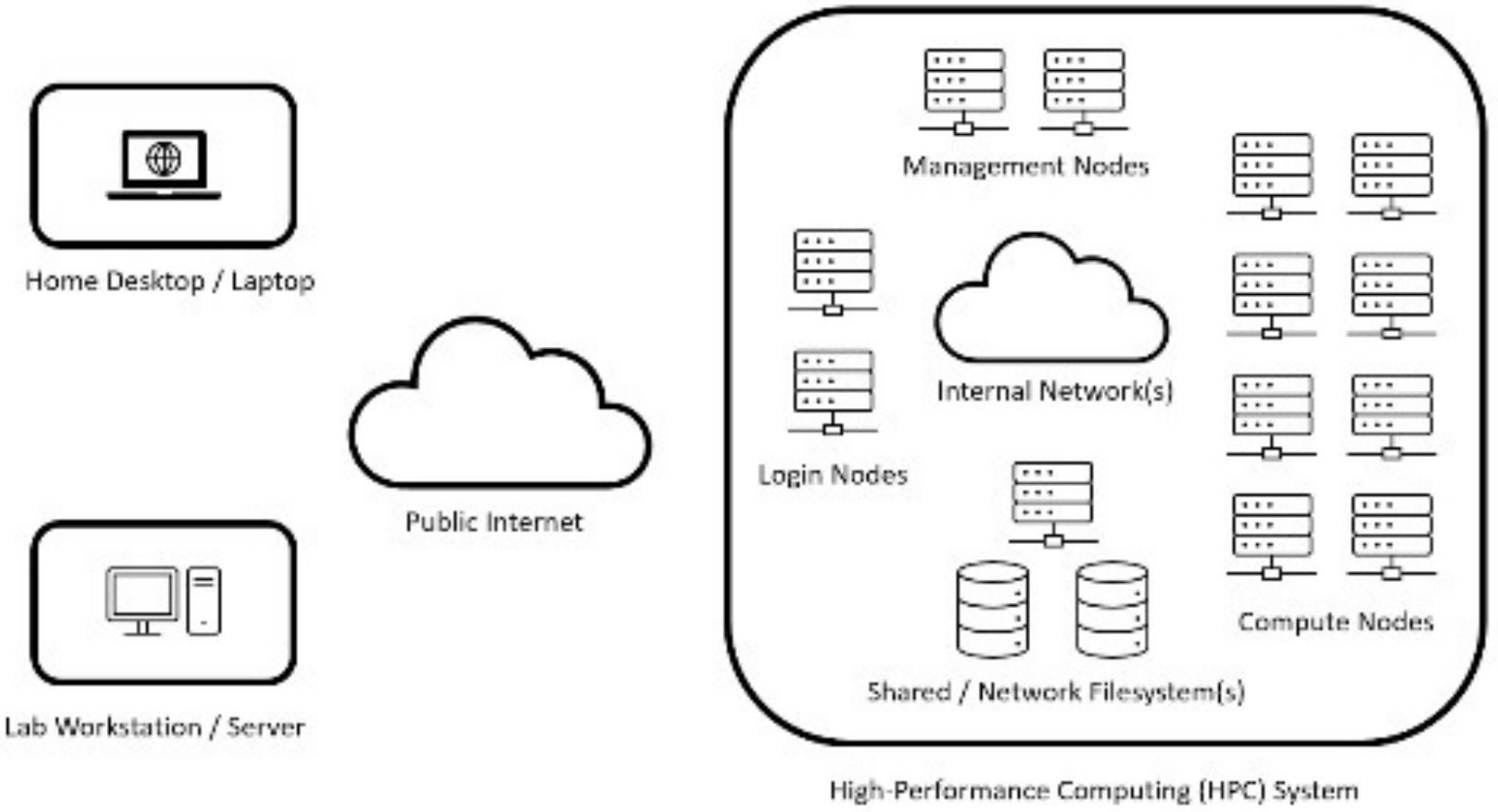
- Use secure connections: when you choose insecure connections your account is vulnerable to hacking
- Use portal.expanse.sdsc.edu



Accessing and Running Secure Notebooks on HPC Systems

- Install notebook application:
  - Locally: install Anaconda on your laptop
  - Remotely:
    - Install Anaconda/conda on the remote machine (default is HTTP) – not recommended
    - Launch securely (HTTPS) using SRPS/`galyleo` -- *`recommended`*
- Running remotely:
  - Connect over HTTP (default, insecure)
  - Connect over HTTP + SSH tunneling (secure, but inconvenient)
  - Connect over HTTPS + using the *Satellite Reverse Proxy Service* (SRPS) and *`galyleo` client (secure, convenient)*
- You can launch Jupyter services on SDSC:
  - CPU and GPUs
  - Interactive nodes: command line
  - Slurm batch script
- Treat the Notebook URL like a Password!

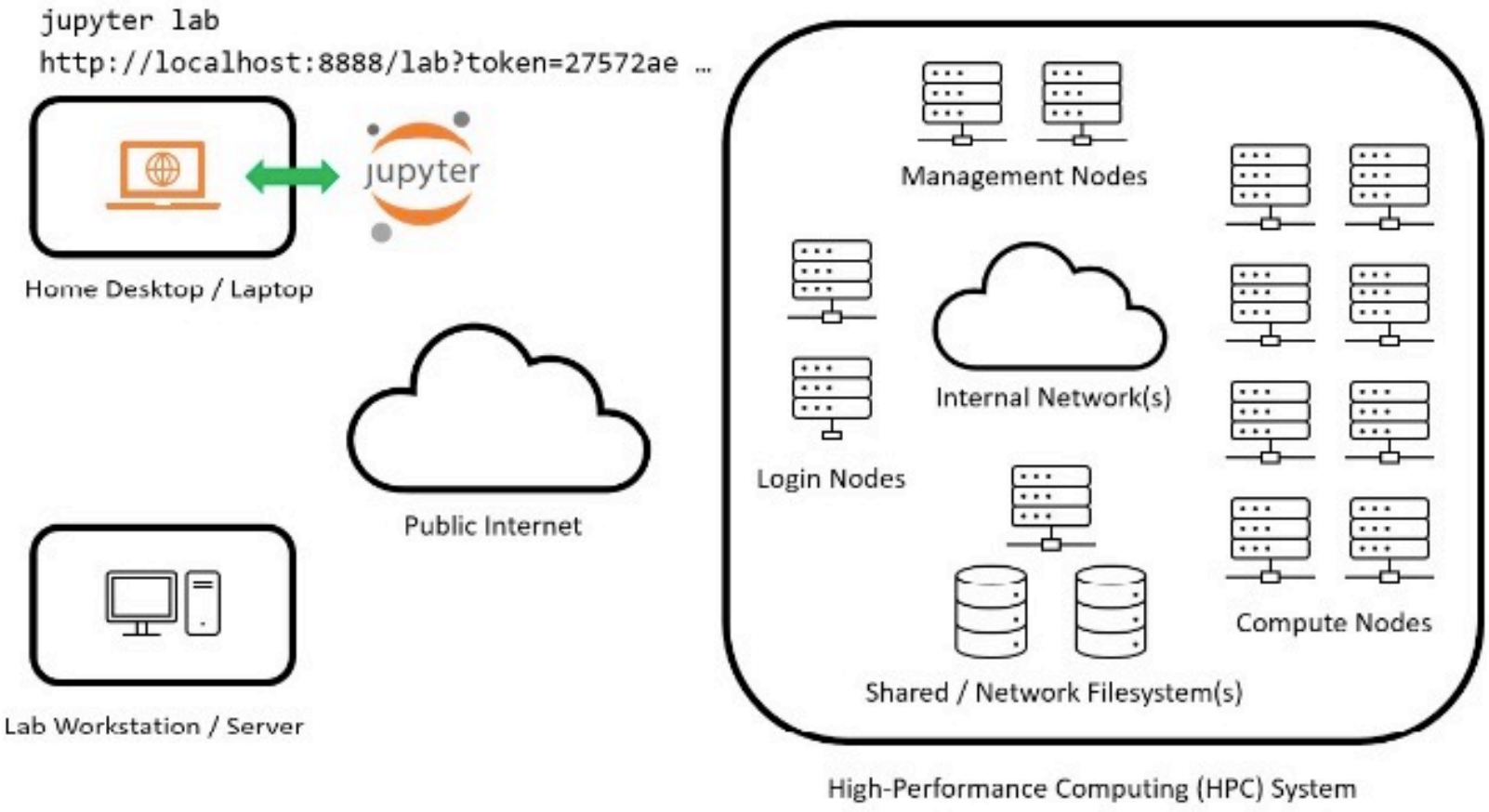
Standard HPC Ecosystem



Src: M Kandes: https://education.sdsc.edu/training/interactive/202112_running_jupyter_notebooks_on_expanse/

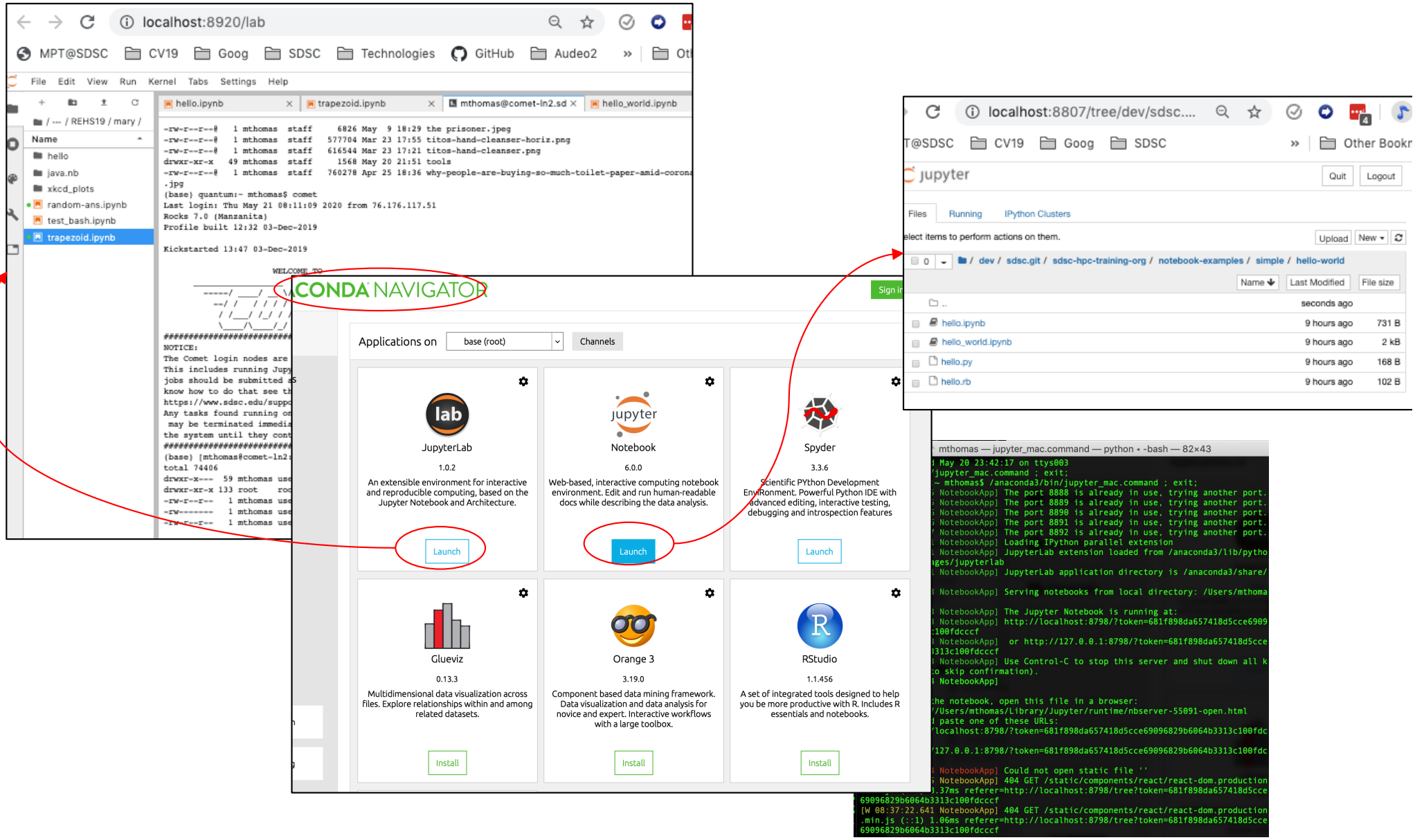
Running Notebooks Locally Over HTTP

Install the Anaconda application and use it to launch your notebooks



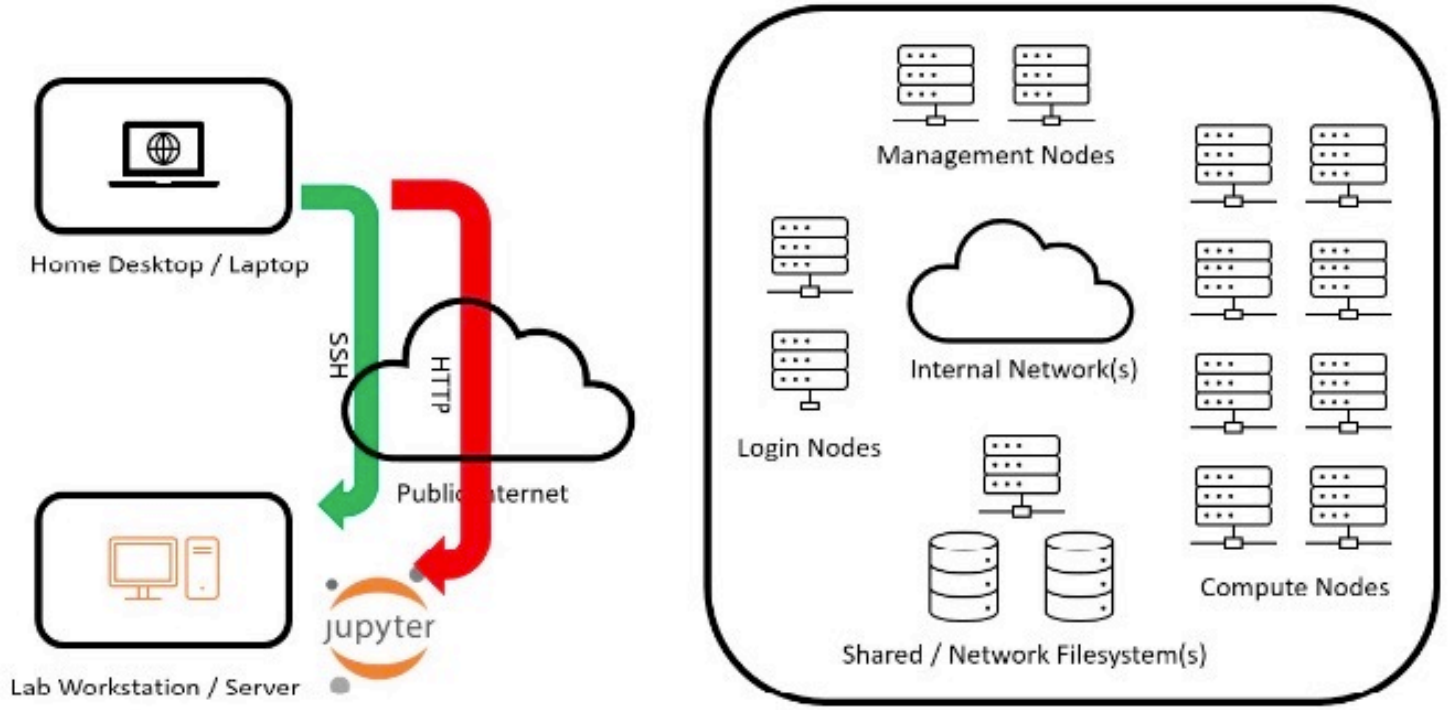
Src: M Kandes: https://education.sdsc.edu/training/interactive/202112_running_jupyter_notebooks_on_expanse/

Anaconda on Local Host or Laptop



Running Notebooks Remotely Over HTTP

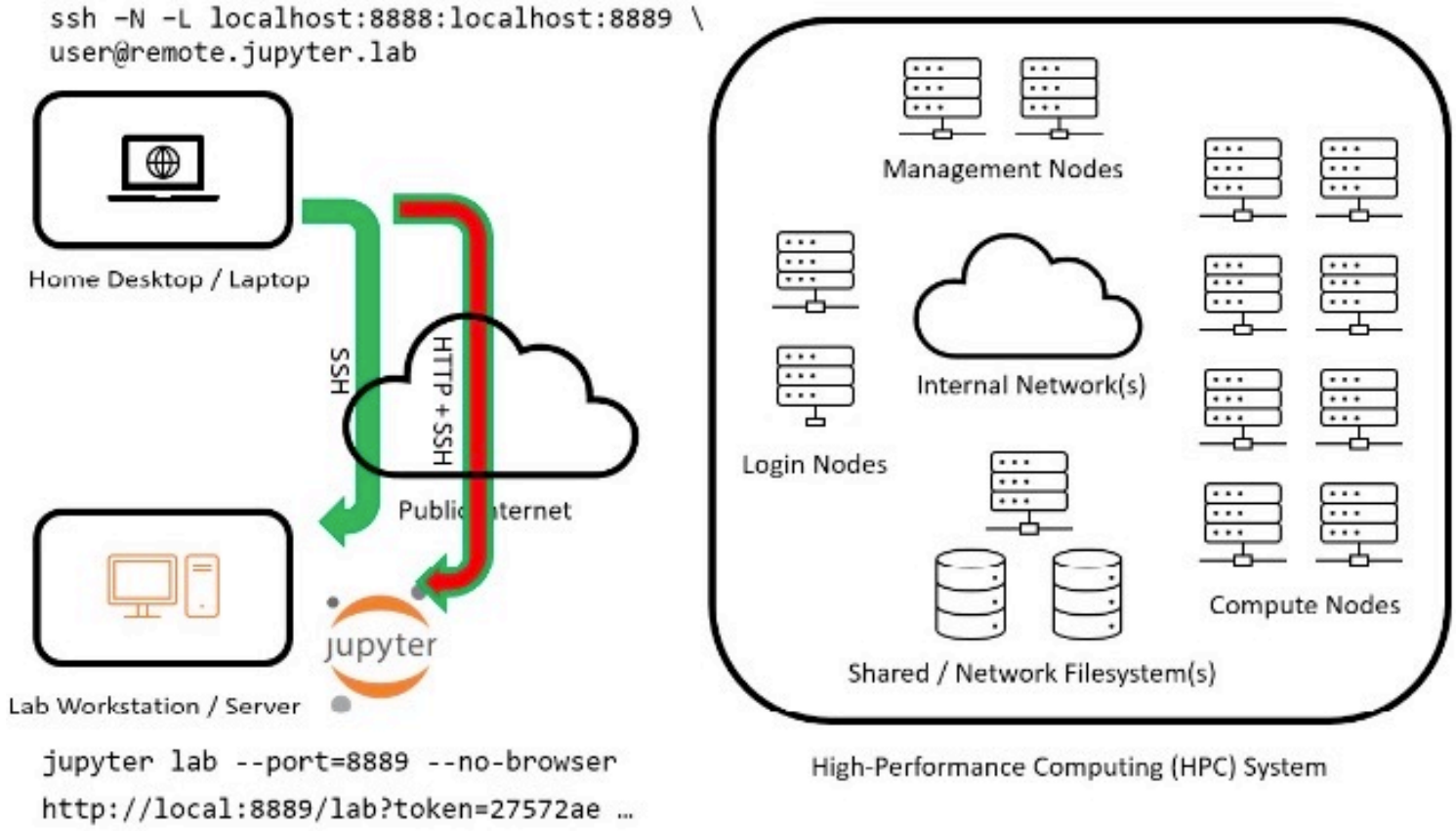
- Messages over HTTP
- Not encrypted
- Vulnerable to hacking



Src: M Kandes: https://education.sdsc.edu/training/interactive/202112_running_jupyter_notebooks_on_expanse/

Running Notebooks Remotely Over HTTP Using SSH Tunneling

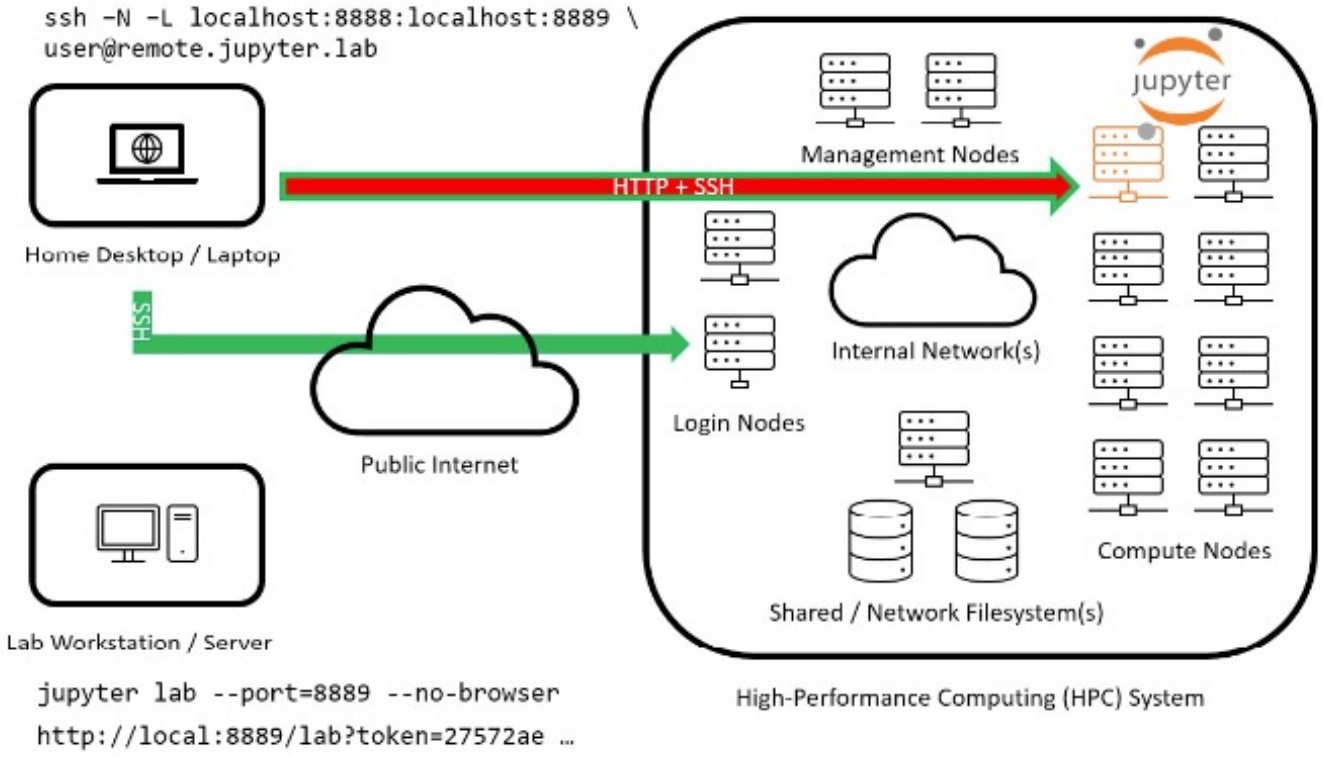
- Notebooks running on Remote host
- Messages over HTTP, but sent via secure tunnel



Src: M Kandes: https://education.sdsc.edu/training/interactive/202112_running_jupyter_notebooks_on_expanse/

Running Notebooks Remotely Over HTTP Using SSH Tunneling on HPC System

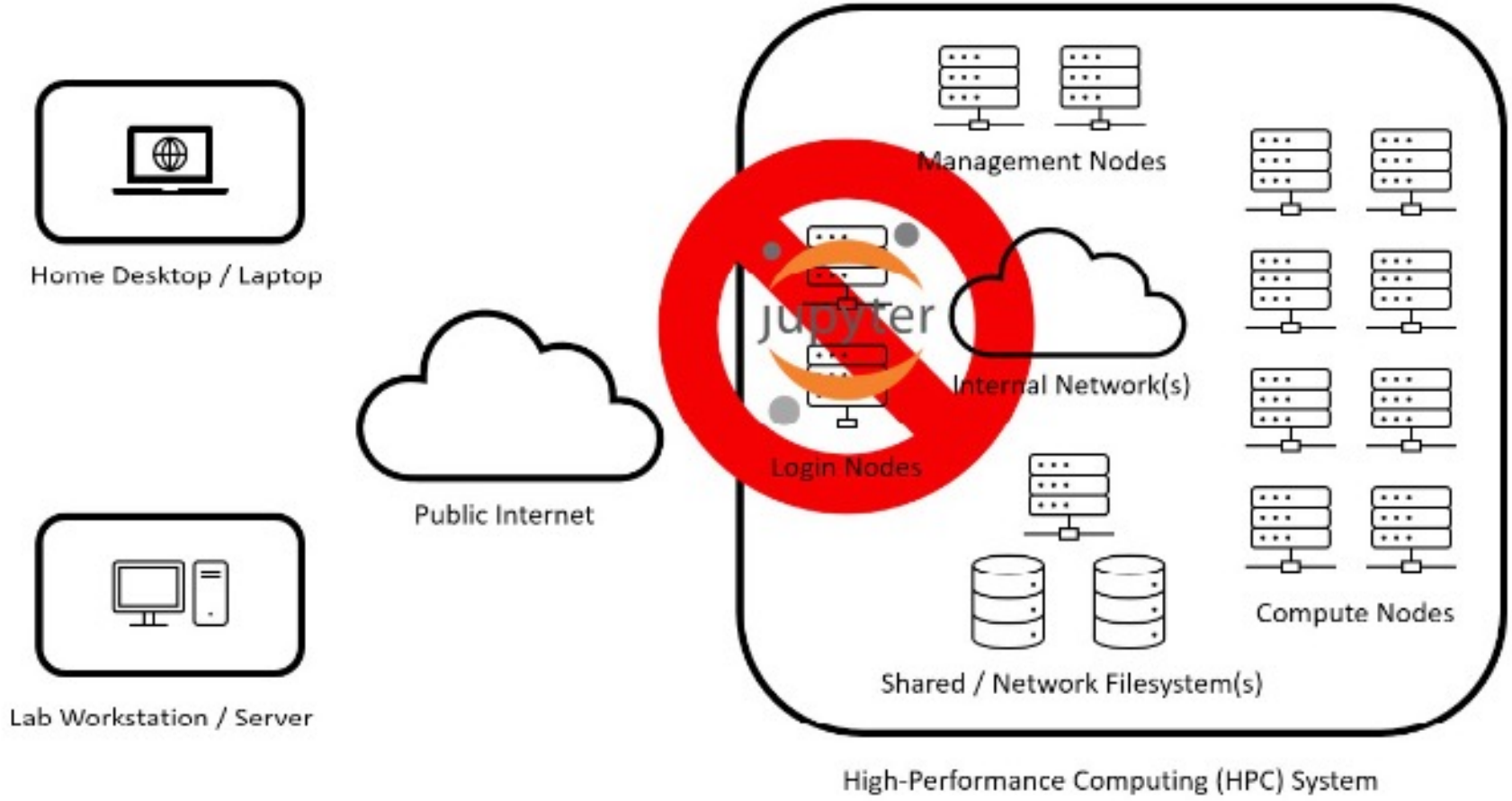
- Notebook running on HPC System
- Messages over HTTP, but passing via secure tunnel
- But do not run on compute nodes!



Src: M Kandes: https://education.sdsc.edu/training/interactive/202112_running_jupyter_notebooks_on_expanse/

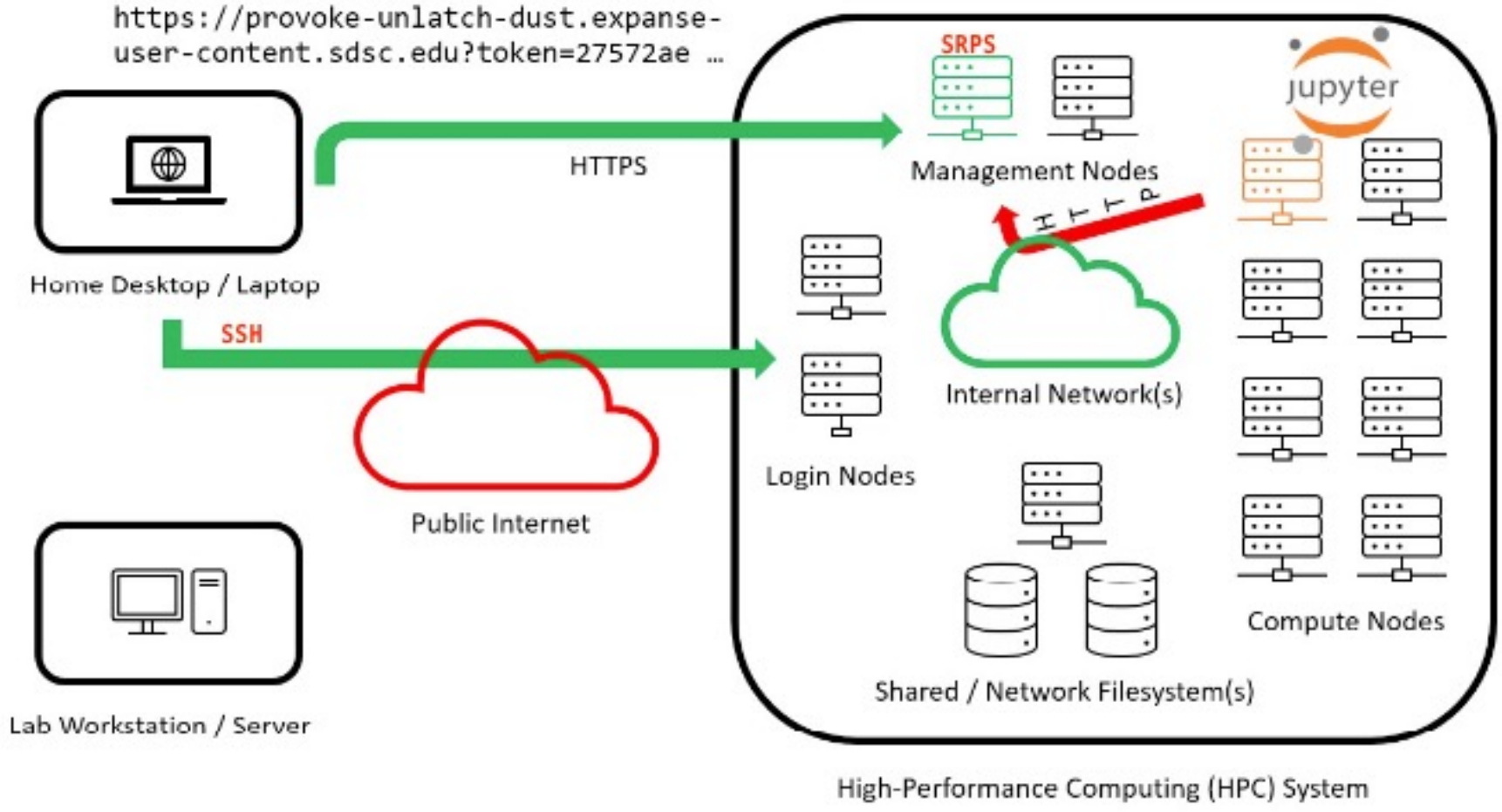
Warning

Do not run notebooks/interactive services on the login nodes!



Src: M Kandes: https://education.sdsc.edu/training/interactive/202112_running_jupyter_notebooks_on_expanse/

Running Notebooks Remotely Using SRPS



Src: M Kandes: https://education.sdsc.edu/training/interactive/202112_running_jupyter_notebooks_on_expanse/

SDSC Satellite Reverse Proxy Service

- SRPS: prototype system that allows users to launch secure standard Jupyter Notebooks on on any Expanse compute node using a reverse proxy server.
  - Notebooks will be hosted on the internal cluster network as an HTTP service using standard Jupyter commands.
  - Service available to the user outside of the cluster firewall over HTTPS connection between the external users web browser and the reverse proxy server.
- Goal: minimize software changes for users, improve security of user notebooks running on SDSC systems.
- SRPS can run on any HPC system capable of supporting Apache on internal network.

galyleo

- 2nd generation shell utility developed to orchestrate a user's interaction with both Satellite and Slurm to start a Jupyter session within a batch job.

- Developed while reviewing start-jupyter (prototype client) codebase to sort out how best to support Expanse (OOD) Portal and HPC User Services Group long-term; integrated into an existing SSH tunneling orchestration utility to use Satellite proxy service instead

- Key features in design:

    - No need to install conda environment or update packages
    - Increases flexibility for users to configure software environment; but also try to makes it simpler for them to do this themselves
    - Batch job script is generated completely on-the-fly.
    - Command-line argument driven.
    - Quiet mode for OOD portal

https://github.com/mkandes/galyleo

Satellite Client: galyleo

Key features in design:

- User calls galyleo.sh launch script, which requests token from Satellite, passes token to batch job script and submits the job to Slurm; token redeemed from batch job once it runs
- Increase flexibility for users to configure software environment; but also try to make it simpler for them to do themselves
- Batch job script is generated completely on-the-fly.
- Command-line argument driven.
- Quiet mode for OOD portal

```
[username@login01 ~]$ galyleo.sh --help
USAGE: galyleo.sh launch [command-line
option] {value}


  command-line option      : value


    -A | --account         :
    -R | --reservation     :
    -p | --partition       :
    -q | --qos             :
    -N | --nodes           :
    -n | --ntasks-per-node :
    -c | --cpus-per-task   :
    -M | --memory-per-node :  GB
    -m | --memory-per-cpu  :  GB
    -G | --gpus            :
       | --gres            :
    -t | --time-limit      :
    -j | --jupyter         :
    -d | --notebook-dir    :
    -r | --reverse-proxy   :
    -D | --dns-domain      :
    -s | --sif             :
    -B | --bind            :
       | --nv              :
    -e | --env-modules     :
       | --conda-env       :
    -Q | --quiet           : 1
```

https://github.com/mkandes/galyleo

Launching CPU notebooks using galyleo

Step 1:
Login and setup user environment

Step 2:
Run command to launch secure notebook

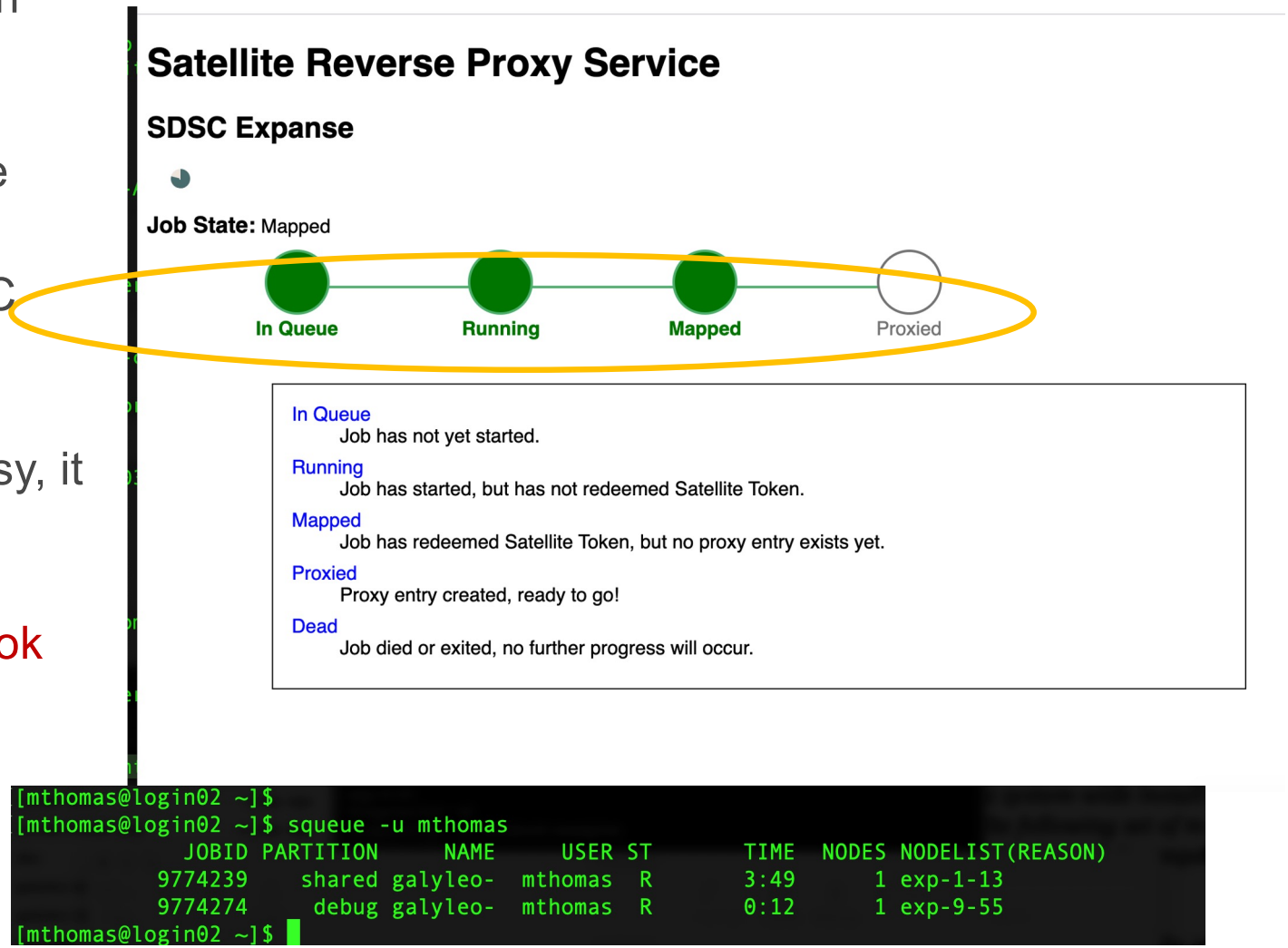
Step 3:
Copy URL; paste into browser on local system

Step 4:
Monitor Slurm queue; wait for job to start

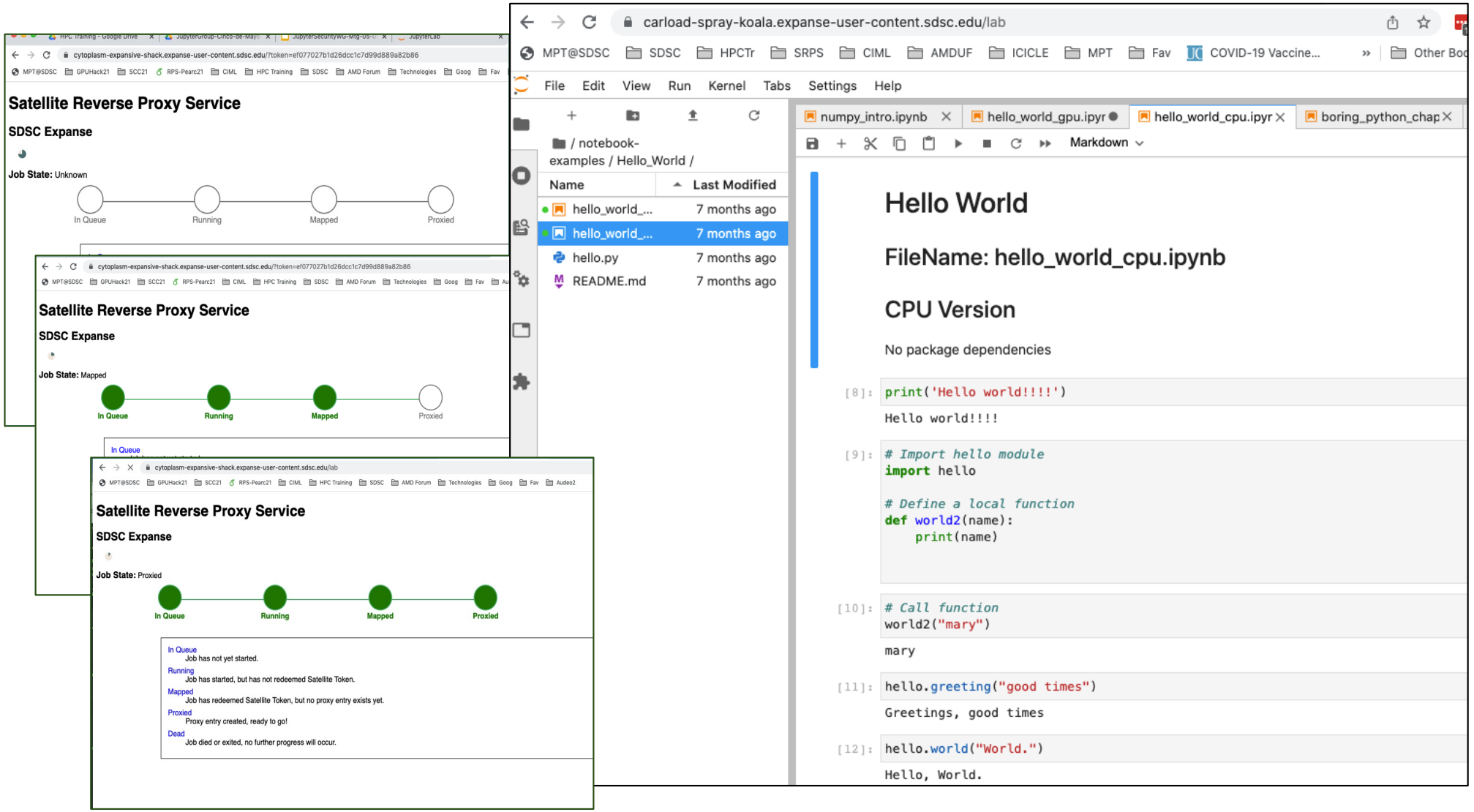
```
[username@login01 ~]$ which galyleo.sh
/usr/bin/which: no galyleo.sh in (/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-
zen/gcc-8.3.1
[SNIP]
home/username/.local/bin:/home/username/bin)
[username@login01 ~]$ export PATH="/cm/shared/apps/sdsc/galyleo:${PATH}"
[username@login01 ~]$ which galyleo
/cm/shared/apps/sdsc/galyleo/galyleo

[username@login01 ~]$ galyleo launch --account use300 --partition shared --cpus 1 --
memory 2 --time-limit 00:30:00 --env-modules cpu,gcc,anaconda3
[snip]
Submitted Jupyter launch script to Slurm. Your SLURM_JOB_ID is 9773665
[snip]
Your Jupyter notebook session will begin once compute resources are allocated to
your job by the scheduler.

https://carload-spray-koala.expanse-user-content.sdsc.edu/lab

[username@login01 ~]$ squeue -u username
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
           9773665 gpu-debug galyleo-  username PD       0:00      1 (None)
[username@login01 ~]$ squeue -u username
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
           9773665 gpu-debug galyleo-  username  R       0:20      1 exp-7-59
```

Satellite Server Pending Page

- Load notebook URL in browser; wait for it to launch
- Monitor pending page
- Run the “squeue” command on the HPC system to check job status
- If the job queue is busy, it may take a while to launch the notebook
- Treat Jupyter Notebook URL as a password!



Satellite Pending Page



Launching GPU notebooks using galyleo

- GPU Notebooks run better when using containers. SDSC maintains several containers on Expanse
- See: /cm/shared/apps/containers/singularity

Step 1:
Login and setup user environment

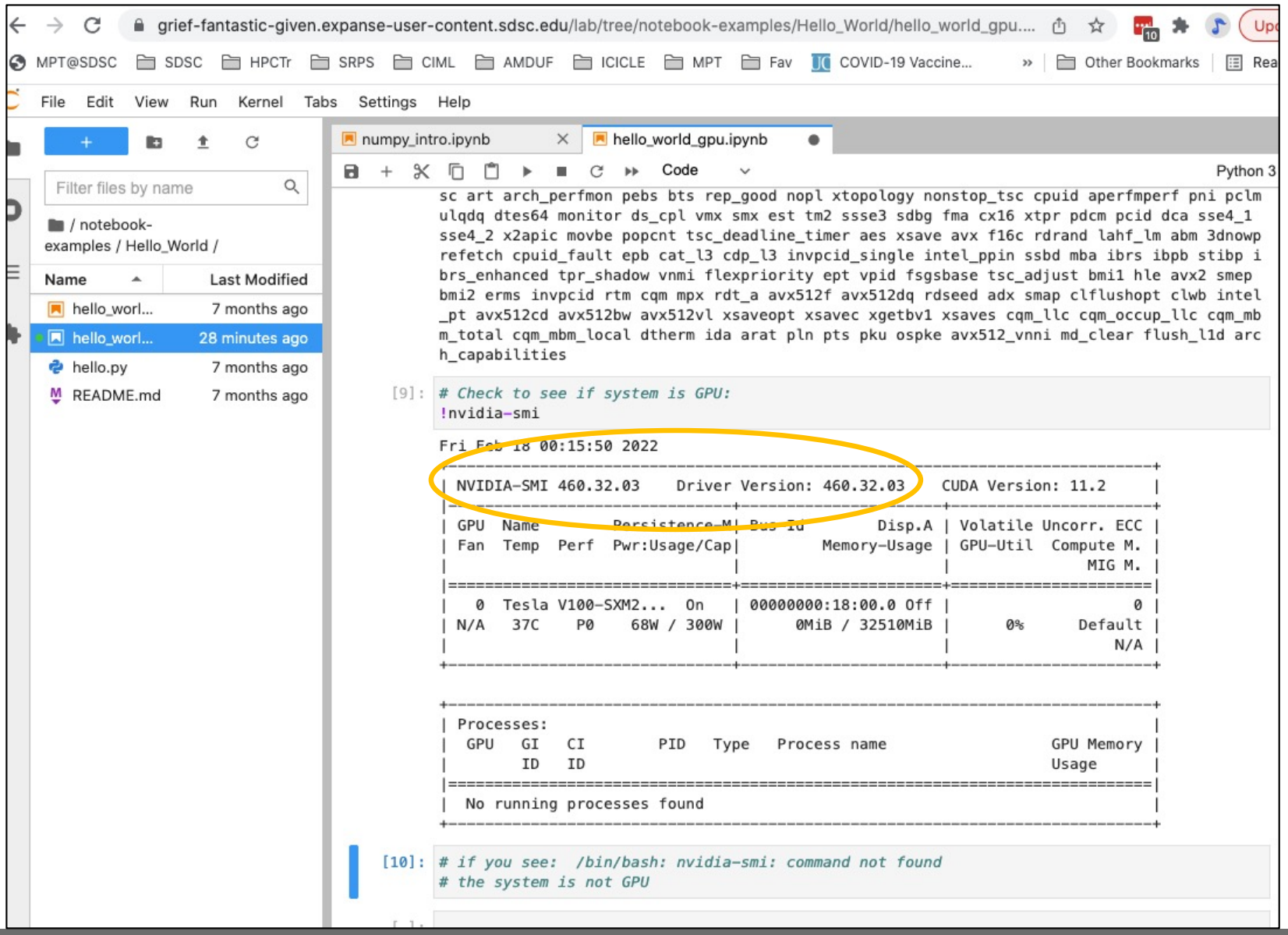
Step 2:
Run command to launch secure notebook

Step 3:
Copy URL; paste into browser on local system

Step 4:
Monitor Slurm queue; wait for job to start

```
[username@login01 ~]$ which galyleo.sh
/usr/bin/which: no galyleo.sh in (/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen/gcc-8.3.1
[SNIP]
home/username/.local/bin:/home/username/bin)
[username@login01 ~]$ export PATH="/cm/shared/apps/sdsc/galyleo:${PATH}"
[username@login01 ~]$ which galyleo
/cm/shared/apps/sdsc/galyleo/galyleo
[username@login01 ~]$ galyleo launch --account use300 --partition gpu-debug --cpus 10 --memory 93 --gpus 1 --time-limit 00:5:00 --env-modules singularitypro --sif /cm/shared/apps/containers/singularity/pytorch/pytorch-latest.sif --bind /expanse,/scratch --nv
[snip]
Submitted Jupyter launch script to Slurm. Your SLURM_JOB_ID is 9773912
[snip]
Your Jupyter notebook session will begin once compute resources are allocated to your job by the scheduler.
https://grief-fantastic-given.expanse-user-content.sdsc.edu?token=5097acb6f32ab82dd51b4524c267d2fd

[username@login01 ~]$ squeue -u username
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
           9773912 gpu-debug galyleo-  username PD       0:00      1 (None)
[username@login01 ~]$ squeue -u username
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
           9773912 gpu-debug galyleo-  username  R       0:20      1 exp-7-59
```

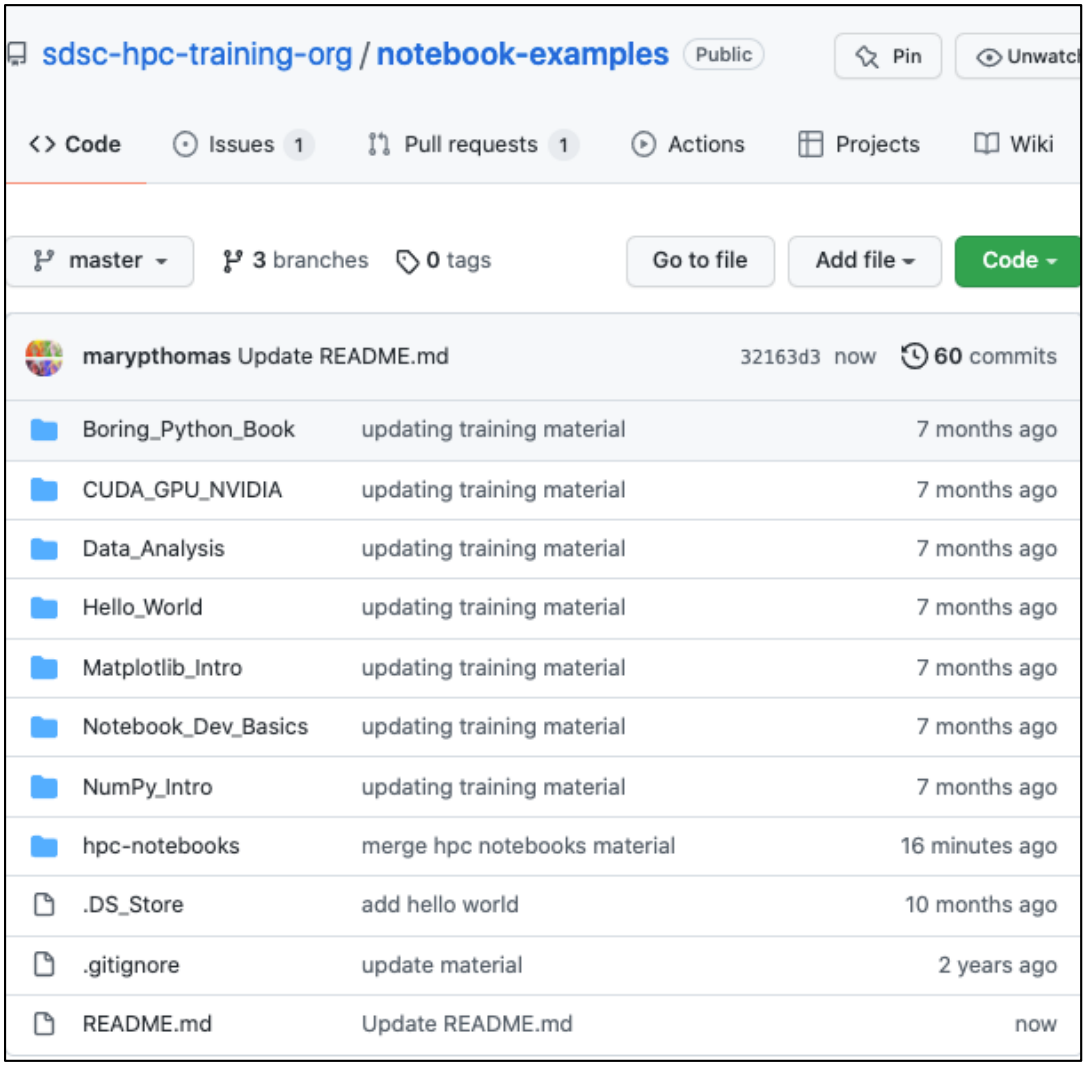
Notebook is launched on GPU device



Notebook Examples

https://github.com/sdsc-hpc-training-org/notebook-examples

- Collection of tested, working notebooks tested on Expanse and other SDSC HPC systems
- Includes range of materials from “hello world” to Spark ML notebooks.
- Note: collection changes often, based on testing and contributions



Resources

- Expanse :
  - Landing page: _expanse.sdsc.edu
  - User Guide: https://expanse.sdsc.edu/support/user_guides/expanse.html
- GitHub Repo for Satellite and Galyleo:
  - https://github.com/sdsc-hpc-training-org/satellite
  - https://github.com/mkandes/galyleo
- SDSC Training Resources
  - https://www.sdsc.edu/education_and_training/training
  - https://github.com/sdsc-hpc-training-org/notebook-examples
- XSEDE Training Resources
  - https://www.xsede.org/for-users/training
  - https://cvw.cac.cornell.edu/expanse/
- Problems? Contact help@xsede.org

Thank You!

if you have problems, please contact help@xsede.org