

# Interactive High-performance (HPC) Computing

COMPLECS Team

<https://bit.ly/COMPLECS>

<https://github.com/sdsc-complecs/interactive-computing/>

**SDSC**  
SAN DIEGO SUPERCOMPUTER CENTER

UC San Diego

## About COMPLECS

COMPLECS (COMPrehensive Learning for end-users to Effectively utilize CyberinfraStructure) is a new SDSC program where training will cover non-programming skills needed to effectively use supercomputers. Topics include parallel computing concepts, Linux tools and bash scripting, security, batch computing, how to get help, data management and interactive computing.

COMPLECS is supported by  
NSF award 2320934.



# Outline

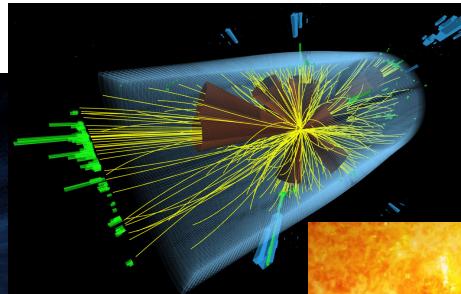
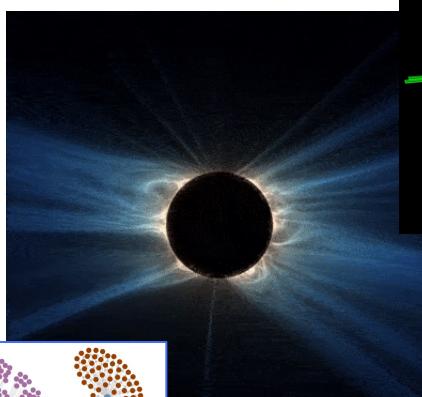
- Defining Interactive HPC
  - High-performance computing (HPC)
  - HPC batch computing
  - Interactive computing
- Accessing Interactive HPC Nodes
  - Launching nodes
  - Running GUIs using X11 forwarding
- Interactive Application Examples
  - Viewing Data: unix file ops (grep, awk, cat), gnuplot, NetCDF
  - Programming & Visualization Platforms: Matlab, R, Jupyter Notebooks
  - Gateways & Portals: simplify access to interactive apps
- Q&A

# You can run amazing jobs on supercomputers!

## Typically parallel or very large memory



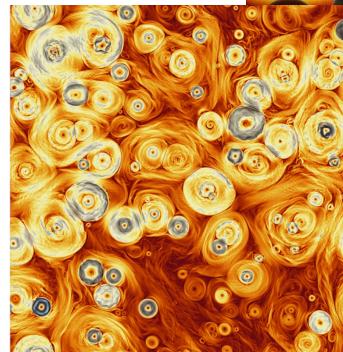
Pelagic fish communities Shapes  
(Jerome Guiet, UCLA)



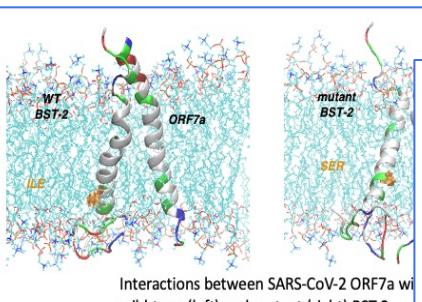
Compact Muon Solenoid (CMS) experiment at the LHC, CERN. Image courtesy of CMS Collaboration; Mc Cauley, Thomas



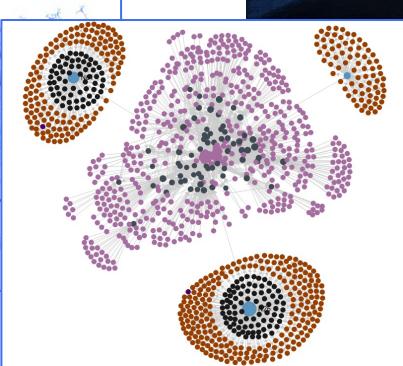
Model of Both Inner and Outer Solar System  
M. S.Clement (Carnegie Institution for Science)



Modeling the sun's corona,  
Alfred Mallet (UC Berkeley)



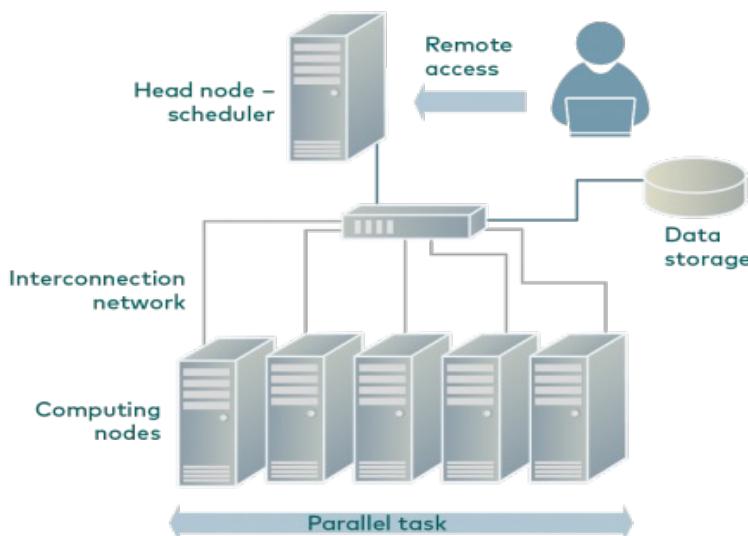
Interactions between SARS-CoV-2 ORF7a with wild-type (left) and mutant (right) BST-2  
Jeff Klauda /U. Maryland



Cooper Downs,  
Predictive Science Inc

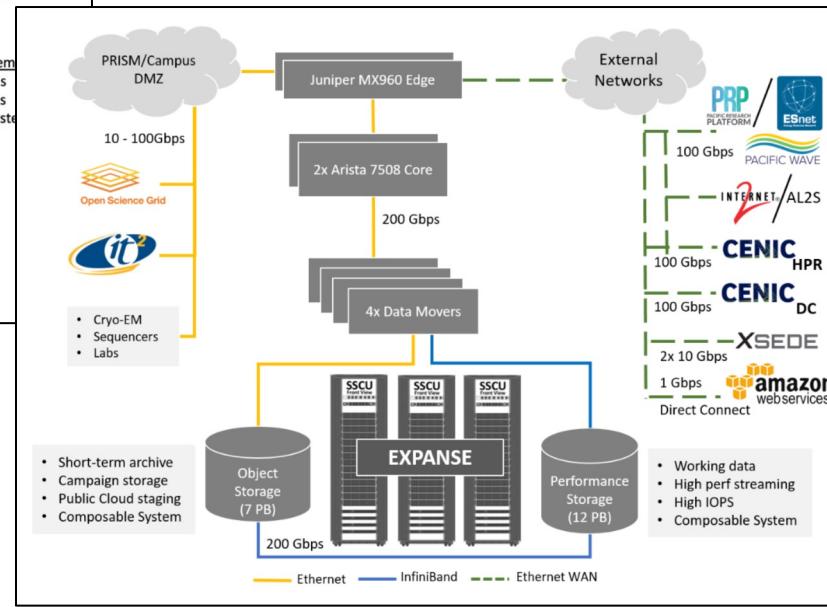
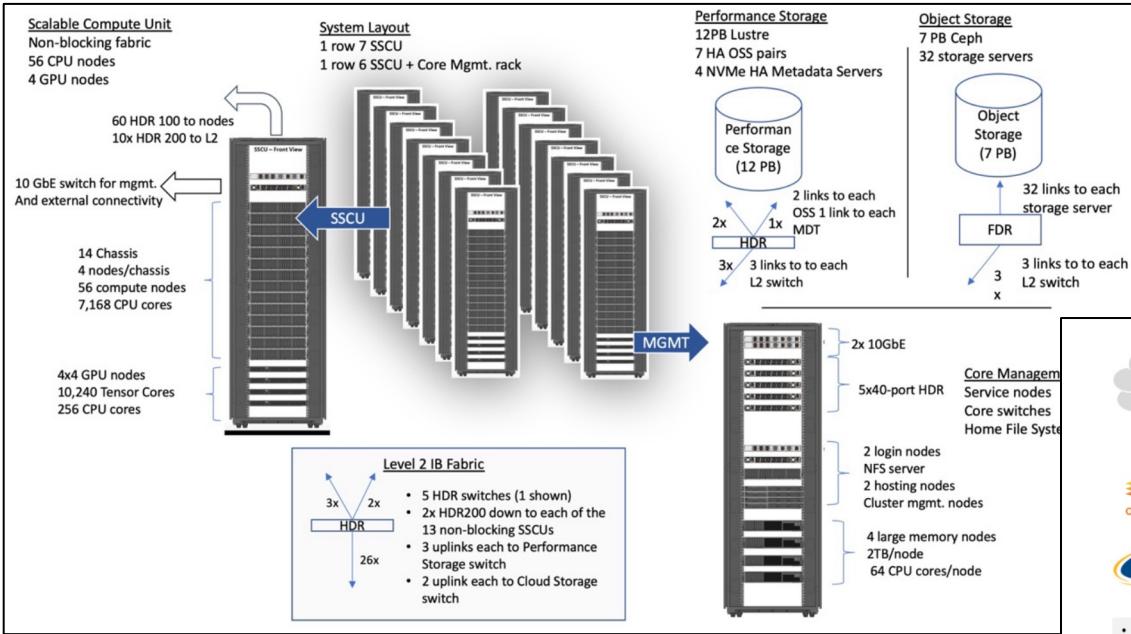
Sample of Internet  
structure from  
CAIDA data (Mark  
Burgess, 12/16/21)

# However, you have to run your jobs on HPC clusters



- Systems powerful but complex
- Jobs can be run from:
  - Command line interface (CLI)
  - The batch queue system
  - Application clients (PyTorch)
- Job scaling:
  - Parallel: 1 core → 1000s of nodes
  - For large jobs, **schedulers** are needed to coordinate tasks

# HPC System Architecture: Expanse @ SDSC



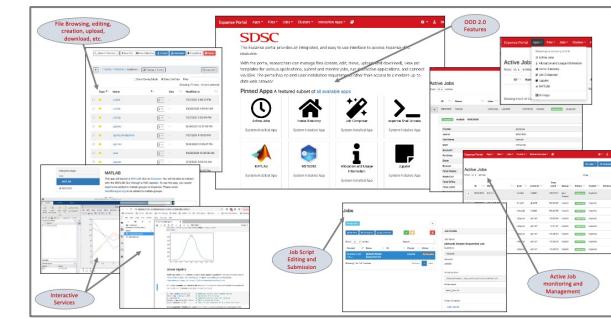
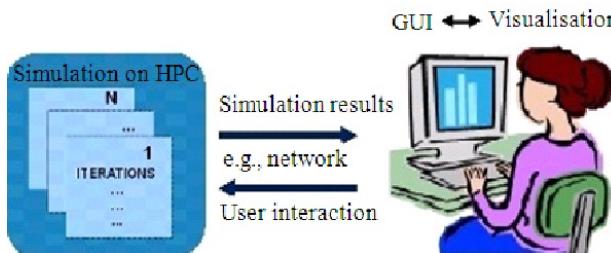
<https://expanse.sdsc.edu>

[https://www.youtube.com/watch?v=uNZyg6X\\_t3s](https://www.youtube.com/watch?v=uNZyg6X_t3s)

<https://access-ci.org>

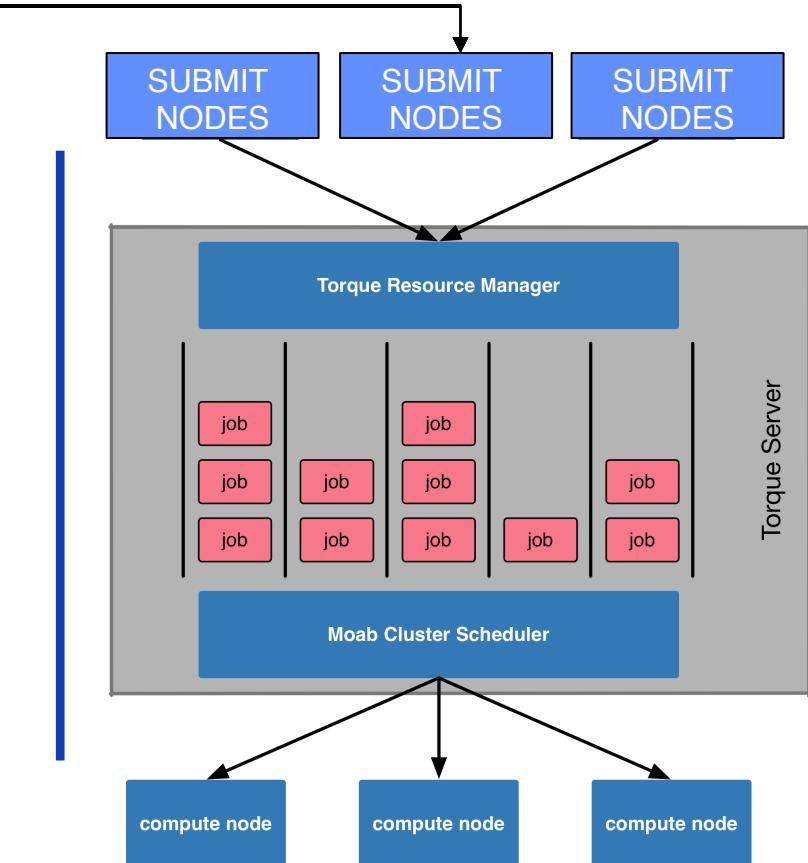
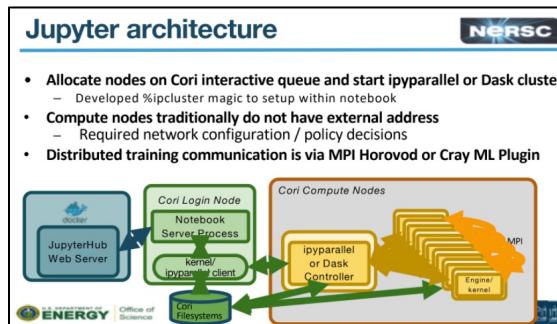
# HPC Jobs can be run as batch jobs (background) or interactively (real time)

Terminal shell – submit batch



<https://portal.expanse.edu>

Interactive Distributed Computing with Jupyter



Src: [https://hpc.dccn.nl/\\_images/torque\\_moab\\_arch.png](https://hpc.dccn.nl/_images/torque_moab_arch.png)

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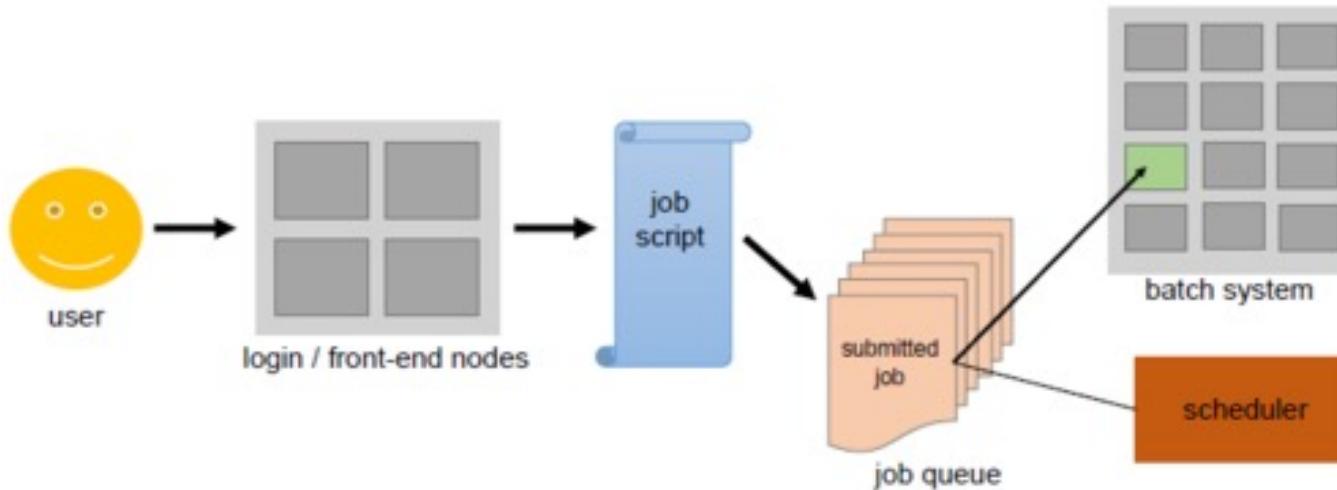
# What is a batch job scheduler & how are they used?

- Any HPC (or HTC) system — usually a cluster of machines — needs a means of **sharing computational resources** fairly between users; without this, there would be anarchy.
- **Batch-queueing systems** — usually abbreviated to simply *batch systems* — are intended to do this.
- All batch systems have at least these features:
  - *a scheduler* for allocating resources (CPUs!) to jobs and for prioritizing jobs;
  - *one or more queues* to which jobs are submitted
  - Job **partitions** (or job queues): queue can be configured for a **particular type of job** (serial or parallel jobs; long or short jobs; or those requiring particularly high memory); members of a group or project).
- You need a basic understanding of batch jobs work in order to run interactive jobs on HPC Clusters (ironic?)

# Batch Scheduler: main goals

- **Minimize time** between job submission and completion:
  - No job should stay in queue for extensive periods of time.
- **Optimize CPU utilization:**
  - Algorithms focus on minimizing CPU idle times.
- **Maximize job throughput:**
  - Manage as many jobs per time unit as possible.
- **Support** running jobs automatically in the background
- **Finalizes jobs:** ensures job data and results are recorded & stored where you want them.

# Simple “Batch Scheduler” Architecture



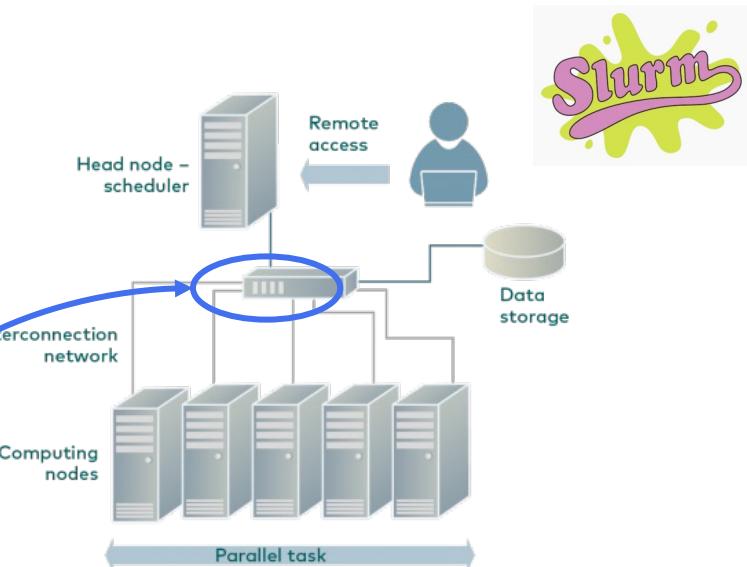
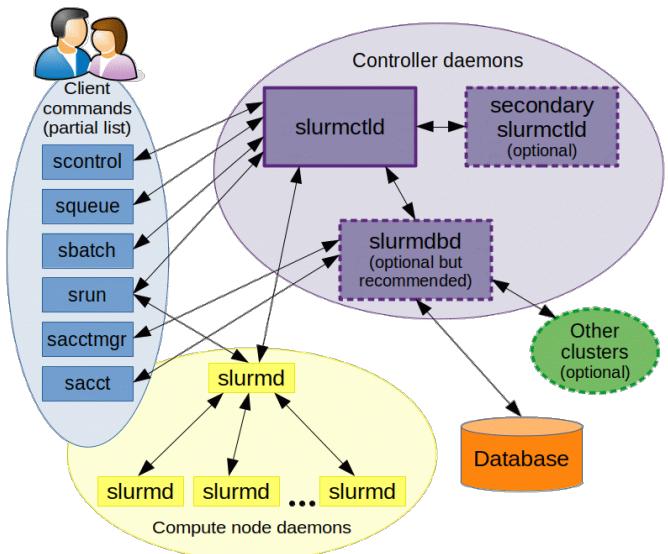
- Batch scheduler: software that implements a *batch system* on a cluster.
- Users do not run calculations interactively -- instead they submit *non-interactive batch jobs* to the *scheduler*.
- All work about the same: some are open source; some cost money; some are very expensive.

[https://hpc-wiki.info/hpc/Scheduling\\_Basics](https://hpc-wiki.info/hpc/Scheduling_Basics)

# Batch jobs: Slurm resource manager

Simple Linux Utility for Resource Management

- Open Source, runs on many systems
- “Glue” for parallel computer to schedule and execute jobs
- Role: Allocate resources within a cluster
  - Nodes (unique IP address)
  - Interconnect/switches
  - Generic resources (e.g. GPUs)
  - Launch and otherwise manage jobs



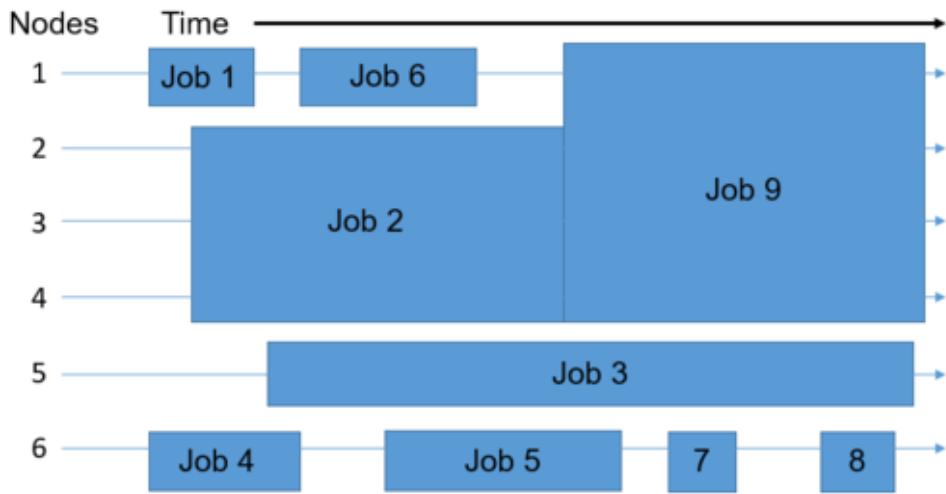
## Functionality:

- Prioritize queue(s) of jobs;
- decide when and where to start jobs;
- terminate job when done;
- Appropriate resources;
- manage accounts for jobs

# How a scheduler schedules jobs

- Simple example:
  - a 6-node system
  - user wants to run 9 jobs.
- Scheduler places the jobs in the queue and then onto the available nodes as they open up.

*Many parameters affect scheduling: number of jobs submitted, required runtime, required number of cores, required main memory, accelerators, libraries, etc.*



**Scheduler needs to play kind of "multidimensional tetris" to fill the cluster's nodes evenly and efficiently.**

[https://hpc-wiki.info/hpc/Scheduling\\_Basics](https://hpc-wiki.info/hpc/Scheduling_Basics)

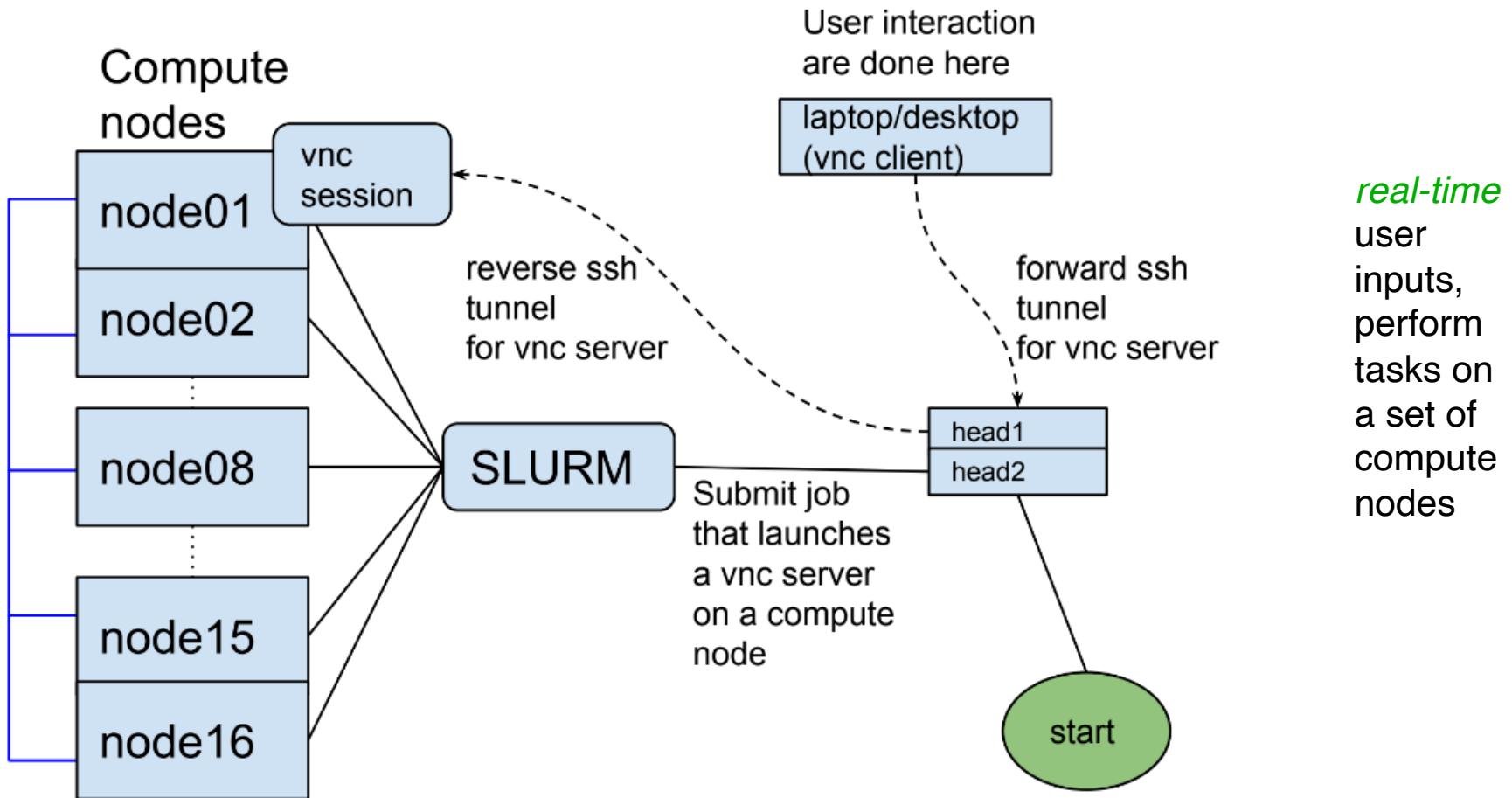
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# What is Interactive HPC Computing

- 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- Motivation

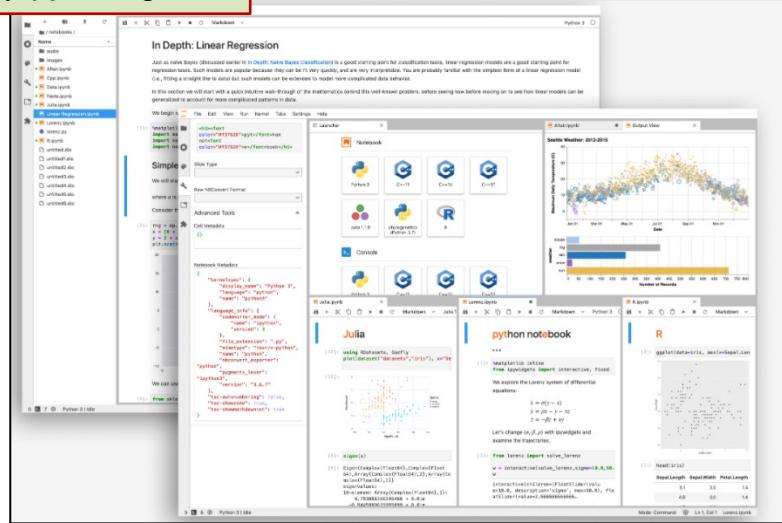
- **Need more memory:** Your jobs no longer fit onto the CPU/system you have been using:
  - That is why Expanse has 768 nodes (128 cores per node), with 256 GB DDR memory on each node
  - My MacBook Pro: 1 node, 8 cores, 16 GB DDR
- **Too much data:** your application needs more room:
  - Expanse has 1TB NVME/node, and 12 PB file system.
  - My MBP: 500 GB, no NVME
- **Your network is too slow:**
  - Expanse has connections to ~ 150GB/sec (or faster) networks
  - My MBP: 300 Mbps download; 11 Mbps upload
  - Bioinfo lab, running analysis on PC: FastQ dataset ~ 500 MB: would need 360+ seconds to upload 1 run.

# Interactive HPC Methods & Applications

- Interact with data after job is done:
  - Unix: query file info, location, output, grep, awk, sed
  - Cat the file contents from batch job or raw data
  - NetCDF data browser
- Plot results:
  - From within the code/model using libraries
  - Command-line driven graphing utility : Gnuplot
- Data visualization apps
  - NetCDF, HPF, TAU, ParaView
  - other
- Data Analysis Platforms: Matlab, R

# Interactive HPC Computing

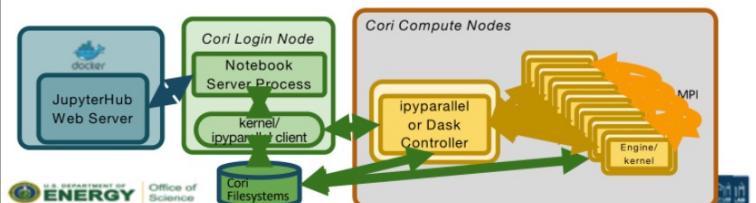
<https://jupyter.org/>



Interactive Distributed Computing with Jupyter (NERSC)

## Jupyter architecture

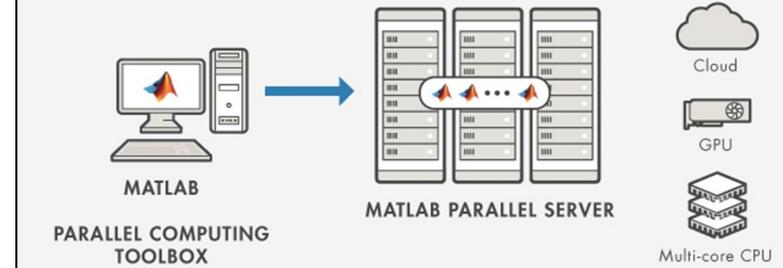
- Allocate nodes on Cori interactive queue and start ipyparallel or Dask cluster
  - Developed %ipcluster magic to setup within notebook
- Compute nodes traditionally do not have external address
  - Required network configuration / policy decisions
- Distributed training communication is via MPI Horovod or Cray ML Plugin



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

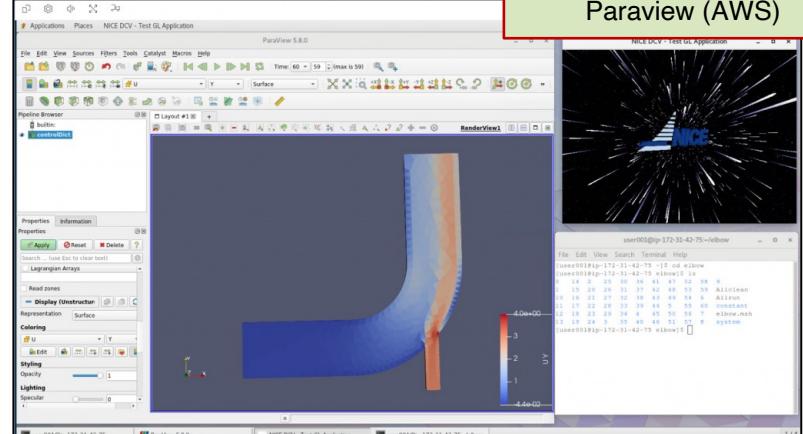
## Parallel Matlab (AWS)

```
>> parpool(parcluster('HPC1'),100);
>> parfor i=1:3000
>> c(i,:) = eig(rand(1000));
>> end
```



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

## Paraview (AWS)



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

# Expanse User Portal

<https://portal.expanse.sdsc.edu>

- Provides Web based access to interactive applications including Jupyter Notebooks & Jupyter Lab, Matlab, Rstudio.
- Access using XSEDE portal account

The image is a composite screenshot of the Expanse User Portal interface, divided into several sections:

- (1) Log onto the Portal:** Shows the main dashboard with links for Jupyter, GPUs, MATLAB, and RSTUDIO.
- (2) Fill out form inputs:** Shows a form for submitting a job, including fields for Account (sdsc54), Partition (gpu), Number of cores (9), and Memory required per node (GB) (9).
- (3) Copy the URL and paste into Web browser:** Shows the URL for the Jupyter session: <https://dipping-ether-pureblood.expanse-user-content.sdsc.edu/token=e5cb92765d875d33875ae>.
- (4) Monitor status window: may take a long time:** Shows the SDSC Expanse status window with four green circles labeled In Queue, Running, Mapped, and Proxied.
- (5) Access your Jupyter Service:** Shows a Jupyter Notebook interface displaying a plot of a bell curve and a section on Linear algebra with code snippets.

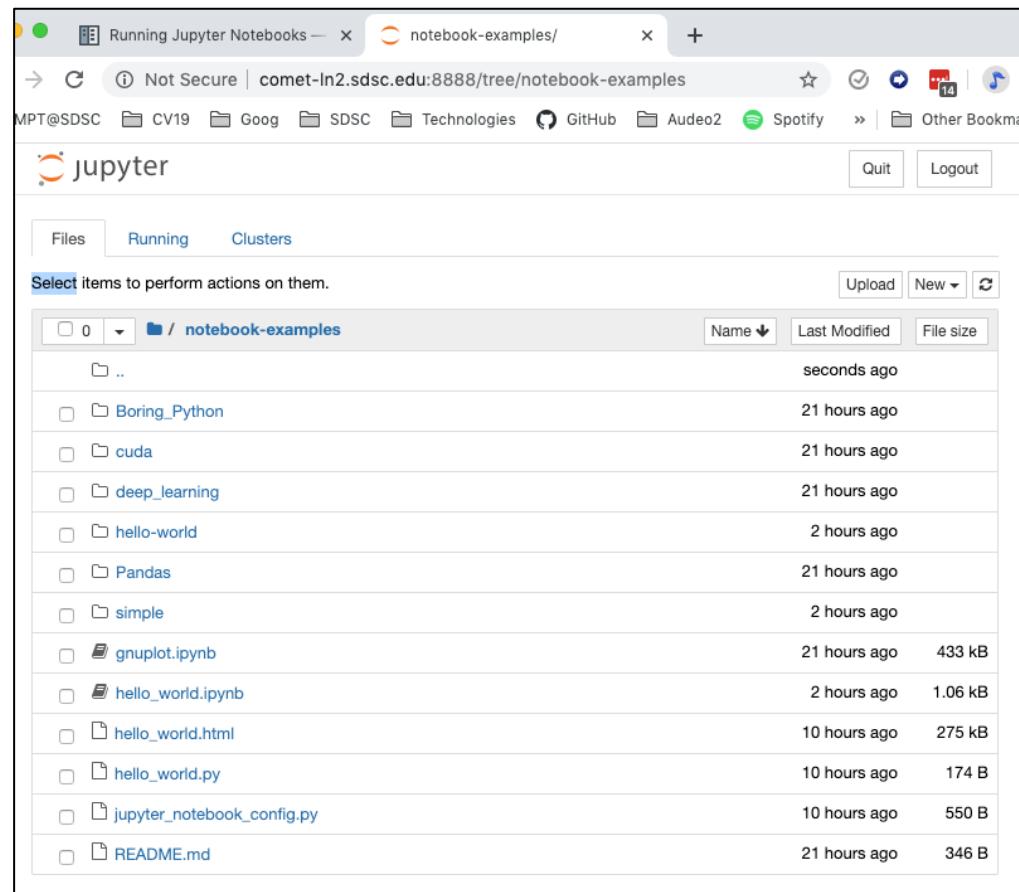
# Interactive Services have a Key Vulnerability: They Provide Access to HPC File Systems, often over HTTP

## 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



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# When would you need to use an Interactive node?

- The application is interactive (Matlab, Notebooks)
- Need to stage large amounts of data
- AI applications (Pytorch, Tensorflow)
- Need to compile a very large, complex application that may take a long time.
  - Java code, 1 million lines, > 30 minutes on DELL 5511 laptop

# Accessing Interactive Compute Nodes on Expanse

- Connect to HPC system (e.g. Expanse) via terminal using SSH → secure connections
- Use the *srun* command to obtain nodes for ‘live,’ command line interactive access:

<b>CPU</b>	<code>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</code>
<b>GPU</b>	<code>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</code>

(Tested 04/17/2024)

# Using An Interactive CPU node

```
[mthomas@login01 calc-prime]$ 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
```

```
srun: job 24457429 has been allocated resources
[mthomas@exp-9-55 calc-prime]$ module purge
[mthomas@exp-9-55 calc-prime]$ module load slurm
[mthomas@exp-9-55 calc-prime]$ module load cpu
[mthomas@exp-9-55 calc-prime]$ module load gcc/10.2.0
[mthomas@exp-9-55 calc-prime]$ module load openmpi/4.1.1
[mthomas@exp-9-55 calc-prime]$ mpirun -n 64 ./mpi_prime
06 August 2023 11:10:26 PM
PRIME_MPI    n_hi= 5000000      C/MPI version
An MPI example program to count the number of primes: #
processes is 64
      N          Pi        Time
      1            0       0.013258
      2            1       0.001058
      4            2       0.000101
      8            4       0.000101
      [SNIP]
     131072      12251     0.110848
     262144      23000     0.410792
     524288      43390     1.527210
    1048576      82025     5.733612
    2097152     155611    21.725862
PRIME_MPI - Master process: Normal end of execution.
06 August 2023 11:12:26 PM
```

Request an interactive node  
for 30 minutes

- Exit interactive session when your work is done or you will be charged more 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 Interactive GPU nodes

```
[snip]
```

```
Last login: Fri Feb 18 12:58:32 2022 from 76.176.117.51
```

```
[username@login02 ~]$
```

```
[username@login02 ~]$ 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
```

```
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              ID   ID   |                    Usage |
+-----+
| No running processes found |
+-----+
```

```
[username@login02 ~]$ exit
```

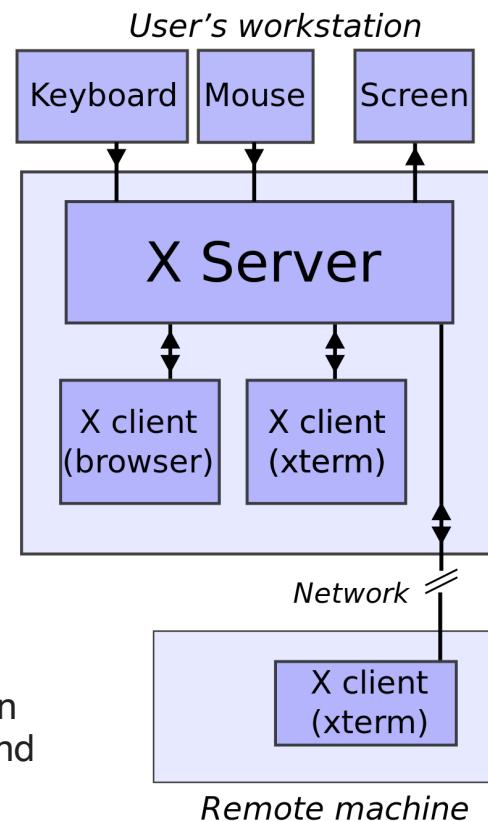
Request an interactive node  
for 30 minutes

Verify you are on a GPU node

Exit when tasks are done

# Visualizing Apps: Use X11 Forwarding

- X Window System (X11): windowing system for bitmap displays, common on Unix-like operating systems.
    - MacOS uses Quartz
  - X is an architecture-independent system for remote graphical user interfaces and input device capabilities
- 
- X server receives input from a local keyboard and mouse and displays to a screen.
  - Web browser and a terminal emulator run on the user's workstation
  - A terminal emulator runs on a remote computer but is controlled and monitored from the user's machine



SRC: [https://en.wikipedia.org/wiki/X\\_Window\\_System](https://en.wikipedia.org/wiki/X_Window_System)

# X11 Forwarding: connecting to Expanse

- On MacOS: Install X11 forwarding software:
  - MacOS: Xquartz
- Use the connection command:

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

```
[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
```

Note: MacOS/Ventura has an X11 problem that is being debugged.

# X11 Forwarding to Expanse Interactive Node

- Create two Expanse X11 login connections  
`ssh -Y mthomas@login.expanse.sdsc.edu`
- Connection #1: request interactive node

```
[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 24457429 has been allocated resources
[mthomas@exp-9-55]$
```

- Connection #2: connect to the interactive node; set up module environment and launch app

```
[mthomas@login01 ~] ssh -Y exp-9-55
Last login: Wed Dec  6 19:21:56 2023 from 10.21.0.19
[mthomas@exp-9-55 ~]$ module load gpu/0.17.3b
[mthomas@exp-9-55 ~]$ module load matlab/2022b/nmbr5dd
[mthomas@exp-9-55 ~]$ matlab
```

Note: MacOS/Ventura has an X11 problem that is being debugged.

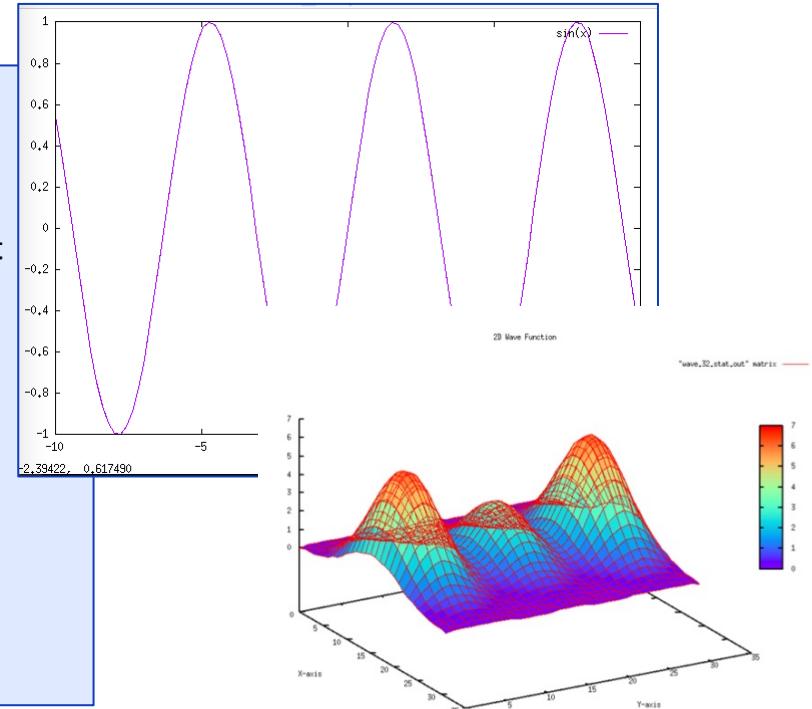
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# gnuplot

- *Depends on X11*
- *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.

```
[mthomas@exp-9-55]$ module load cpu/0.17.3b gcc/10.2.0/npcyll4
[mthomas@exp-9-55~]$ module load gnuplot/5.4.2/mfnpvw
[mthomas@exp-9-55]$ which gnuplot
/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen2/gcc-
10.2.0/gnuplot-5.2.8-uwugzxg4dgxaiciheiengol67cw7m6yg/bin/gnuplot
[mthomas@exp-9-55]$ 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>
```



# NetCDF

- 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
- Similar to high-density format (HDF)
- NetCDF clients (ncview, ncdump) can be used to query and plot data in real-time

NCdump Variable Data

Variable: humidity(0:9:1, 0:4:1)

NCdump Image Write

```
float humidity(station=10, time=5);
:standard_name = "specific_humidity";
:coordinates = "time lat lon alt";

data:
{
    {1.0, 2.0, 3.0, 4.0, 5.0},
    {6.0, 7.0, 8.0, 9.0, 10.0},
    {11.0, 12.0, 13.0, 14.0, 15.0},
    {16.0, 17.0, 18.0, 19.0, 20.0},
    {21.0, 22.0, 23.0, 24.0, 25.0},
    {26.0, 27.0, 28.0, 29.0, 30.0},
    {31.0, 32.0, 33.0, 34.0, 35.0},
    {36.0, 37.0, 38.0, 39.0, 40.0},
    {41.0, 42.0, 43.0, 44.0, 45.0},
    {46.0, 47.0, 48.0, 49.0, 50.0}
}
```



<https://unidata.ucar.edu/netcdf>

# Configuring NetCDF on Expanse

NetCDF: A tool for viewing binary output data file contents

- Example below is for very simple, serial example provided by SciNet (Canada): see
  - Select the right module environment: it's a big software system
- Set up modules
- Put SciNet ENV vars into bash scripts
- Build the compile command (Makefile not easy to adapt)
- Example will generate a data.nc file
- Browse & query file contents

# NetCDF: Configure Shell Environment

- Add environment variables to your shell env:

```
[mthomas@login02 netcdf]$ cat ~/.bash_profile
[SNIP]
# netcdf library and include paths
SCINET_NETCDF_INC=/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen2/intel-
19.1.1.217/netcdf-c-4.7.4-62xm3fwd6soo2zqqbd4t7jza4ro5riyv/include
SCINET_NETCDF_LIB=/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen2/intel-
19.1.1.217/netcdf-c-4.7.4-62xm3fwd6soo2zqqbd4t7jza4ro5riyv/lib

#HDF5 library and include paths
SCINET_HDF5_INC=/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen2/intel-
19.1.1.217/hdf5-1.10.7-jsee7cinki6pcunimgfe3ovv6lz7gwnt/include
SCINET_HDF5_LIB=/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen2/intel-
19.1.1.217/hdf5-1.10.7-jsee7cinki6pcunimgfe3ovv6lz7gwnt/lib

#update path to binaries
PATH=$PATH:/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen2/intel-
19.1.1.217/netcdf-c-4.7.4-
62xm3fwd6soo2zqqbd4t7jza4ro5riyv/bin:/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-
zen2/intel-19.1.1.217/hdf5-1.10.7-
jsee7cinki6pcunimgfe3ovv6lz7gwnt/bin:/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-
zen2/intel-19.1.1.217/ncview-2.1.8-bm3tockq6ljgtxefovxia5hujnqmpdpn/bin
[SNIP]
```

# NetCDF: Configure Modules

- Setup the right modules for the version you want to use:

```
[mthomas@login02 netcdf]$  
[mthomas@login02 netcdf]$ module load cpu/0.15.4 intel/19.1.1.217 mvapich2/2.3.4  
[mthomas@login02 netcdf]$ module load netcdf-c/4.7.4  
[mthomas@login02 netcdf]$  
[mthomas@login02 netcdf]$  
[mthomas@login02 netcdf]$ which ncdump  
/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen2/intel-19.1.1.217/netcdf-c-4.7.4-  
62xm3fwd6soo2zqqbd4t7jza4ro5riyv/bin/ncdump  
[mthomas@login02 netcdf]$ which ncview  
/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen2/intel-19.1.1.217/ncview-2.1.8-  
bm3tockq6ljqtxefovxia5hujnqmpdpn/bin/ncview
```

# Query NetCDF Data File Contents: ncdump

```
[mthomas@login02 netcdf]$ pwd
[mthomas@login02 netcdf]$ pwd
/home/mthomas/hpcctr-examples/netcdf/parIO/netcdf
[mthomas@login02 netcdf]$ ls *.c
-rw-r--r-- 1 mthomas use300 8874 Oct  5 2010 2darray.c
-rwxr-xr-x 1 mthomas use300 304648 Dec  6 01:27 2darray-simple.c
-rw-r--r-- 1 mthomas use300 15903 Oct  6 2010 parallel2darray.c
-rw-r--r-- 1 mthomas use300 5865 Oct  5 2010 read2darray-simple.c
-rw-r--r-- 1 mthomas use300 240176mpicc -I/cm/shared/apps/spack/cpu/opt/spack/linux-
centos8-zen2/intel-19.1.1.217/netcdf-c-4.7.4-62xm3fwd6soo2zqqbd4t7jza4ro5riyv/include
-L/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen2/intel-19.1.1.217/netcdf-c-
4.7.4-62xm3fwd6soo2zqqbd4t7jza4ro5riyv/lib -lnetcdf -o 2darray 2darray.c
Dec  6 01:27 data-simple.nc
[mthomas@login02 netcdf]$ ./2darray
[mthomas@login02 netcdf]$ ll *.nc
-rw-r--r-- 1 mthomas use300 241164 Dec  6 01:25 data.2darray.nc
-rw-r--r-- 1 mthomas use300 241164 Dec  6 21:27 data.nc
```

# Query NetCDF Data File Contents: ncdump

Tool for viewing output data file contents

```
[mthomas@login02 netcdf]$ ncdump -h
ncdump [-c|-h] [-v ...] [[-b|-f] [c|f]] [-l len] [-n name] [-p n[,n]] [-k] [-x] [-s]
[-t|-i] [-g ...] [-w] [-Ln] file
[-c]          Coordinate variable data and header information
[-h]          Header information only, no data
[-v var1[,...]] Data for variable(s) <var1>, ... only
[-b [c|f]]    Brief annotations for C or Fortran indices in data
[-f [c|f]]    Full annotations for C or Fortran indices in data
[-l len]      Line length maximum in data section (default 80)
[-n name]     Name for netCDF (default derived from file name)
[-p n[,n]]    Display floating-point values with less precision
[-k]          Output kind of netCDF file
[-s]          Output special (virtual) attributes
[-t]          Output time data as date-time strings
[-i]          Output time data as date-time strings with ISO-8601 'T' separator
[-g grp1[,...]] Data and metadata for group(s) <grp1>, ... only
[-w]          With client-side caching of variables for DAP URLs
[-x]          Output XML (NcML) instead of CDL
[-Xp]         Unconditionally suppress output of the properties attribute
[-Ln]         Set log level to n (>= 0); ignore if logging not enabled.
file         Name of netCDF file (or URL if DAP access enabled)
```

# Read NetCDF Data File Contents: ncdump

- Tool for viewing output data file contents

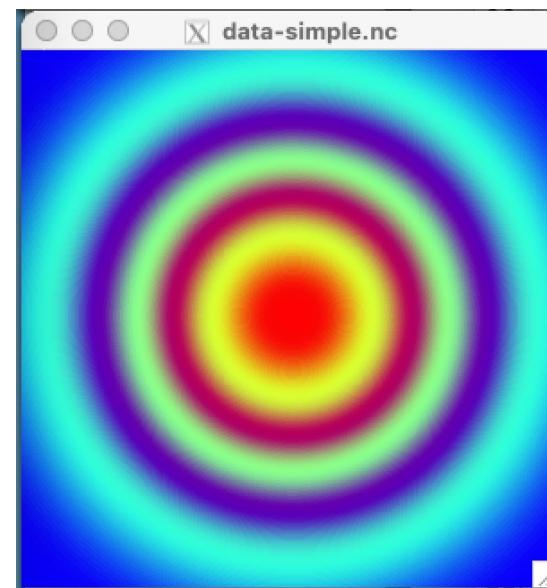
```
[mthomas@login02 netcdf]$ ll *.nc
-rw-r--r-- 1 mthomas use300 241164 Dec  6 01:25 data.2darray.nc
-rw-r--r-- 1 mthomas use300 240176 Dec  6 01:27 data-simple.nc
[mthomas@login02 netcdf]$ ncdump -h data-simple.nc
netcdf data-simple {
dimensions:
X = 100 ;
Y = 100 ;
velocity\ component = 2 ;
variables:
double Density(X, Y) ;
double Velocity(velocity\ component, X, Y) ;
}
[mthomas@login02 netcdf]$ ncdump -x data-simple.nc
<?xml version="1.0" encoding="UTF-8"?>
<netcdf xmlns="http://www.unidata.ucar.edu-namespaces/netcdf/ncml-2.2"
location="data-simple.nc">
  <dimension name="X" length="100" />
  <dimension name="Y" length="100" />
  <dimension name="velocity component" length="2" />
  <variable name="Density" shape="X Y" type="double">
    </variable>
  <variable name="Velocity" shape="velocity component X Y" type="double">
    </variable>
</netcdf>
```

# Read NetCDF Data File Contents: ncdump

```
[mthomas@login02 netcdf]$ ncdump -t data-simple.nc | more
netcdf data-simple {
dimensions:
X = 100 ;
Y = 100 ;
velocity\ component = 2 ;
variables:
double Density(X, Y) ;
double Velocity(velocity\ component, X, Y) ;
data:
Density =
1.07326255555494, 1.07930091286413, 1.08569972700294, 1.09246679805167,
1.09960871294202, 1.10713070597055, 1.11503651964736, 1.12332826729031,
1.13200629886235, 1.14106907162359, 1.1505130272287, 1.16033247694148,
1.17051949666066, 1.18106383345281, 1.19195282526666, 1.20317133545959,
1.21470170369791, 1.22652371469942, 1.23861458616838, 1.25094897713016,
1.26349901770561, 1.27623436117604, 1.28912225897801, 1.30212765903751,
1.31521332760545, 1.3283399944956, 1.34146652135377, 1.35455009230782,
1.3675464260648, 1.38041000823913, 1.39309434241745, 1.40555221819654,
[SNIP]
-2.8468704354508, -2.69398173507181, -2.54522816466233,
-2.40084389414749, -2.2610296301804, -2.12595326718743,
-1.99575075552494, -1.87052716603845, -1.75035792940546,
-1.63529022805598, -1.52534451818797, -1.42051615941371,
-1.32077712986823, -1.22607780516019, -1.13634878032523, -1.05150271492394 ;
```

# Visualize NetCDF Data: ncview

```
[mthomas@login02 netcdf]$ ll *.nc
-rw-r--r-- 1 mthomas use300 241164 Dec  6 01:25 data.2darray.nc
-rw-r--r-- 1 mthomas use300 240176 Dec  6 01:27 data-simple.nc
[username@login02 netcdf] ncview data-simple.nc
```



# Outline

- What is High-Performance Computing (HPC)?
- What is HPC batch computing
- Defining Interactive HPC Computing
- Accessing Interactive HPC Nodes
- Interactive Application Examples
  - Viewing Data: unix file operators (grep, awk, cat), gnuplot, NetCDF
  - Programming & Visualization Platforms: Matlab, R, Jupyter Notebooks
  - Gateways & Portals: simplify access to interactive apps

# Expanse Interactive Jobs: Running Matlab with GU

```
[mthomas@login01 ~]$ 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  
srun: job 14833549 queued and waiting for resources  
srun: job 14833549 has been allocated resources  
[mthomas@exp-9-55 ~]$ module load gpu/0.17.3b  
[mthomas@exp-9-55 ~]$ module load matlab/2022b/nmbr5dd  
[mthomas@exp-9-55 ~]$ module list  
Currently Loaded Modules:  
 1) shared                 3) sdsc/1.0           5) gpu/0.17.3b      (g)  
 2) slurm/expanse/21.08.8   4) DefaultModules    6) matlab/2022b/nmbr5dd
```

Check that you have the right modules loaded

```
[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)  <-- nothing happens  
>>
```

Run GUI app from another connection using the -Y flag  
(see earlier X11 slides)

# Expanse Interactive Jobs: Running 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 Windows, see: <http://systems.eecs.tufts.edu/x11-forwarding/>

**Step 1:** Log on to Expanse, using **-Y** option (trusted); create two connections

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

**Step 2: Window 1:** Request an interactive node, using **srun command**

This window will not be used for anything else but holding the interactive node connection

```
[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 26814162 queued and waiting for resources
srun: job 26814162 has been allocated resources
[mthomas@exp-9-55 ~]$
```

**Step 3: Window 2:**  
Connect to the interactive node: **atlab**

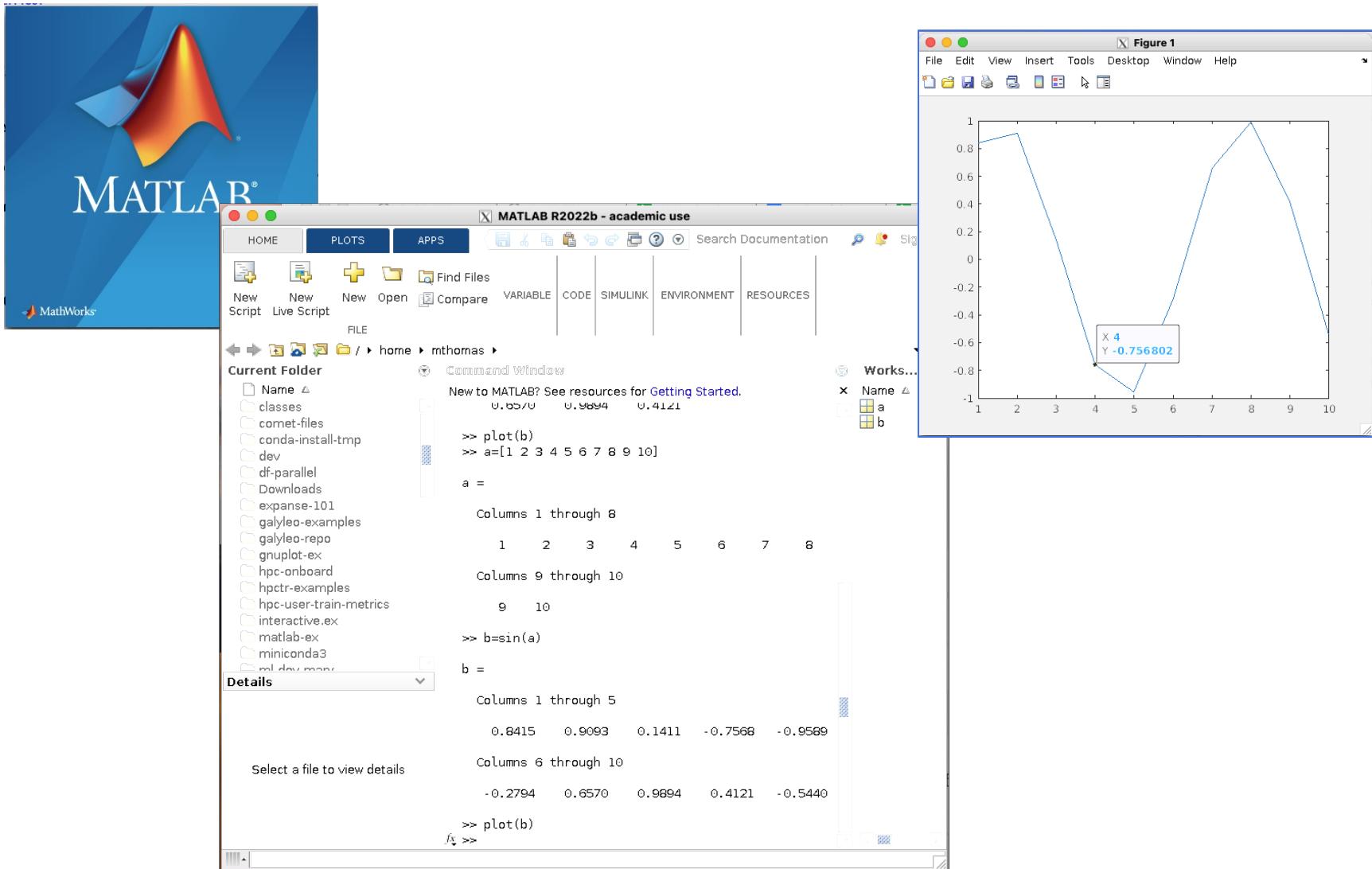
```
[mthomas@login02 ~]$ ssh -Y exp-9-55
Last login: Wed Dec 6 19:23:47 2023 from 10.21.0.19
```

**Step 4: Window 2:**  
Setup Matlab module environment  
Launch Matlab

GUI:  
**USE EXPANSE PORTAL**

```
[mthomas@exp-9-55 ~]$ module load gpu/0.17.3b
[mthomas@exp-9-55 ~]$ module load matlab/2022b/nmbr5dd
[mthomas@exp-9-55 ~]$ module list
Currently Loaded Modules:
 1) shared           3) sdsc/1.0      5) gpu/0.17.3b (g)
 2) slurm/expanse/21.08.8   4) DefaultModules    6)
matlab/2022b/nmbr5dd
[mthomas@exp-9-55 ~]$ matlab
MATLAB is selecting SOFTWARE OPENGL rendering.
```

# HPC Interactive Jobs: Running Matlab with GUI



# Outline

- What is High-Performance Computing (HPC)?
- What is HPC batch computing
- Defining Interactive HPC Computing
- Accessing Interactive HPC Nodes
- Interactive Application Examples
  - Viewing Data: unix file operators (grep, awk, cat), gnuplot, NetCDF
  - Programming & Visualization Platforms: Matlab, R, Jupyter Notebooks
  - Gateways & Portals: simplify access to interactive apps

# TSCC Interactive Jobs: Running R console (no GUI)

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

```
[mthomas@tscc-login2 ~]$ qsub -l -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*

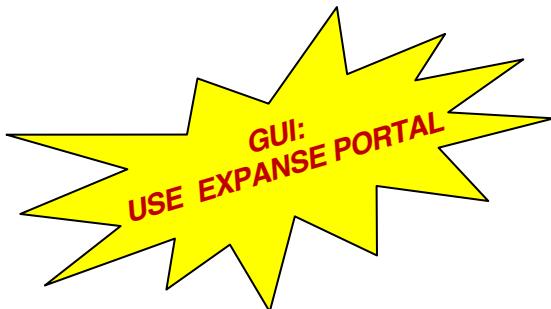
```
[mthomas@tscc-4-46 ~]$ module load R
Unloading compiler-dependent module openmpi_ib/3.1.4
[mthomas@tscc-4-46 ~]$ R
R version 4.0.2 (2020-06-22) -- "Taking Off Again"
Copyright (C) 2020 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)
```

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!"
>
```



# Outline

- Defining Interactive HPC
  - High-performance computing (HPC)
  - HPC batch computing
  - Interactive computing
- Accessing Interactive HPC Nodes
  - Launching nodes
  - Running GUIs using X11 forwarding
- Interactive Application Examples
  - Viewing Data: unix file ops (grep, awk, cat), gnuplot, NetCDF
  - Programming & Visualization Platforms: Matlab, R, **Jupyter Notebooks**
  - Gateways & Portals: simplify access to interactive apps
- Q&A

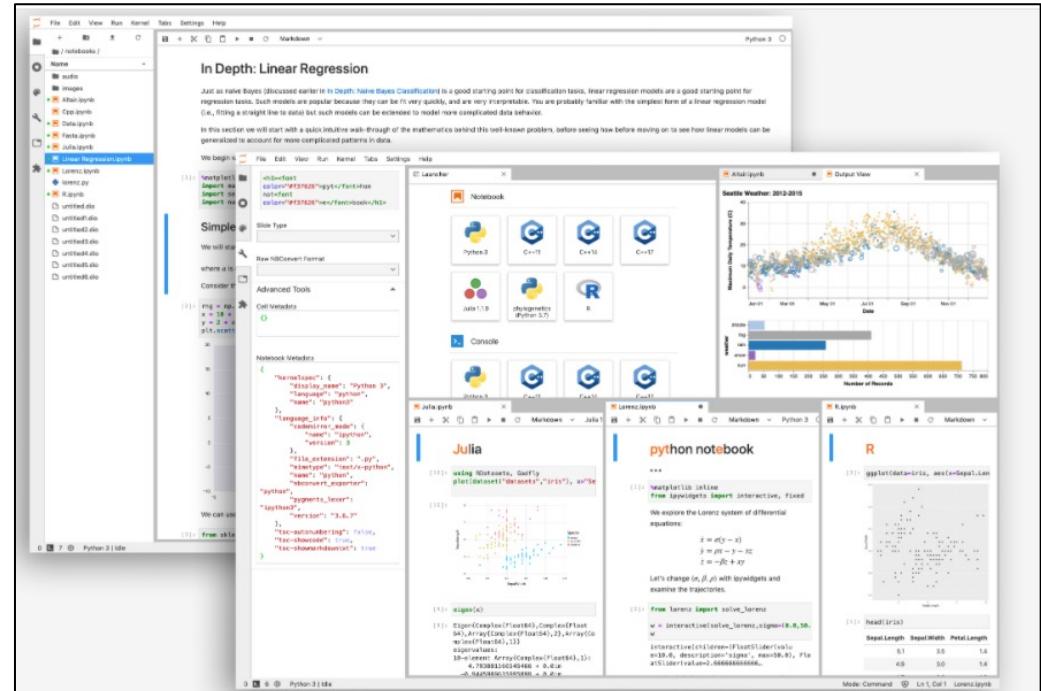
# Jupyter Notebooks

## 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



# Accessing and Running Secure Notebooks on SDSC HPC Systems

- Install notebook application:
  - Locally: install Anaconda on your laptop
  - Remotely:
    - Install Anaconda/conda on the remote machine (**default is HTTP**) – not 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:
  - Launch securely (HTTPS) using SRPS/*galyleo* -- **recommended**
  - CPU and GPUs
  - Interactive nodes: command line *or* Slurm batch script
- **Treat the Notebook URL like a Password!**

# SDSC Satellite Reverse Proxy Service

- SRPS: prototype system that allows users to launch secure standard Jupyter Notebooks 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.

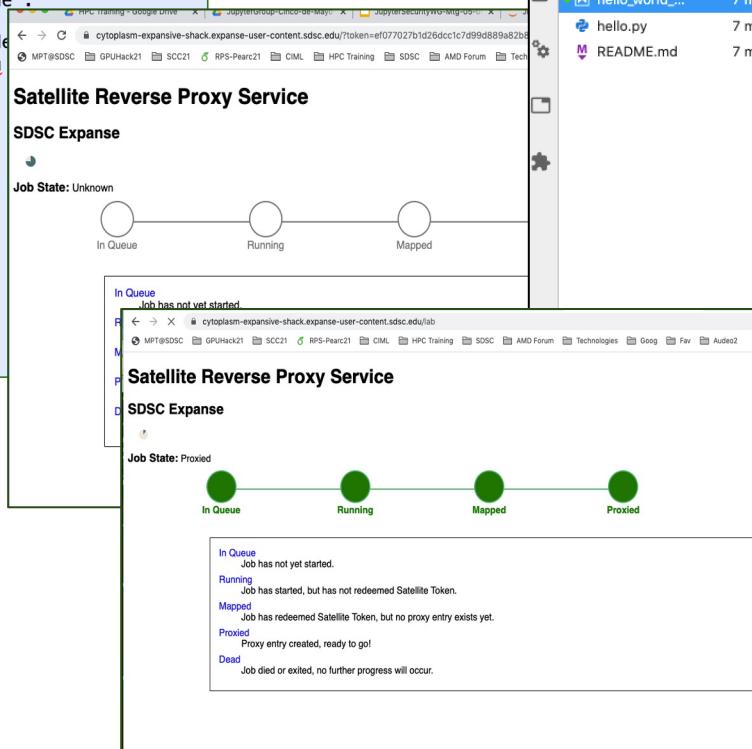
# galyleo

- 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:
  - HTTPS URL
  - Supports containers (Singularity on Expanse) → **GPU environment**
  - 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-Galileo System

```
[username@login01 ~]$ export  
PATH="/cm/shared/apps/sdsc/galileo:$PATH"  
  
[username@login01 ~]$ galileo.sh --help  
USAGE: galileo.sh launch [command-line  
option] {value}  
command-line option      : value  
-A | --account          :  
-R | --reservation       :  
-P | --partition         :  
-Q | --gpus              :  
-N | --nodes              :  
-n | --ntasks_per_node   :  
-C | --cpus_per_task     :  
-M | --memory_per_node   :  
-m | --memory_per_cpu    :  
-G | --gres               :  
-t | --time_limit         :  
-j | --jupyter             :  
-d | --notebook_dir        :  
-r | --reverse_proxy       :  
-D | --dns_domain         :  
-s | --sif                 :  
-B | --bind                :  
-nv | --nv                  :  
-e | --env_modules         :  
--conda-env              :  
-Q | --quiet               :
```



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

File Edit View Run Kernel Tabs Settings Help

numpy\_intro.ipynb   hello\_world\_gpu.ipynb   hello\_world\_cpu.ipynb   boring\_python\_chap.ipynb

**Hello World**

**FileName: hello\_world\_cpu.ipynb**

**CPU Version**

No package dependencies

```
[ 8]: print('Hello world!!!!')
Hello world!!!!
```

```
[ 9]: # Import hello module
import hello

# Define a local function
def world2(name):
    print(name)
```

```
[10]: # Call function
world2("mary")
mary
```

```
[11]: hello.greeting("good times")
Greetings, good times
```

```
[12]: hello.world("World.")
Hello, World.
```

# 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 ~] export PATH="/cm/shared/apps/sdsc/galyleo:${PATH}"  
[username@login01 ~]$ 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 galileo

## 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 galileo.sh  
/usr/bin/which: no galileo.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/galileo:${PATH}"  
[username@login01 ~]$ which galileo  
/cm/shared/apps/sdsc/galileo/galileo  
[username@login01 ~]$ galileo launch --account abc123 --partition shared --cpus 2  
--memory 4 --time-limit 00:30:00 --env-modules cpu/0.17.3b,anaconda3/2021.05  
[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 galileo- username PD 0:00 1 (None)  
[username@login01 ~]$ squeue -u username  
JOBID PARTITION NAME USER ST TIME NODES  
NODELIST(REASON)  
9773665 gpu-debug galileo- username R 0:20 1 exp-7-59
```

# Satellite Server Status/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 Reverse Proxy Service

SDSC Expanse

Job State: Mapped

In Queue  
Job has not yet started.

Running  
Job has started, but has not redeemed Satellite Token.

Mapped  
Job has redeemed Satellite Token, but no proxy entry exists yet.

Proxied  
Proxy entry created, ready to go!

Dead  
Job died or exited, no further progress will occur.

```
[mthomas@login02 ~]$ [mthomas@login02 ~]$ squeue -u mthomas
      JOBID PARTITION      NAME      USER ST      TIME  NODES NODELIST(REASON)
      9774239    shared galileo-  mthomas R      3:49      1 exp-1-13
      9774274    debug galileo-  mthomas R      0:12      1 exp-9-55
[mthomas@login02 ~]$
```

# 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

```
[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 1  
--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]
```

Step 2:  
Run command to  
launch secure  
notebook

```
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
```

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

```
[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
```

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

# Verify notebook launched on GPU device

MPT@SDSC File Edit View Run Kernel Tabs Settings Help

numpy\_intro.ipynb X hello\_world\_gpu.ipynb •

Python 3

```
sc art arch_perfmon pebs rep_good nopl xtopology nonstop_tsc cpuid aperfmpf perfmon_pni pclm ulldq dtes64 monitor ds_cpl vmx smx est tm2 ssse3 sdbg fma cx16 xptr pdcm pcid dca sse4_1 sse4_2 x2apic movbe popcnt tsc_deadline_timer aes xsave avx f16c rdrand lahf_lm abm 3dnowp refetch cpuid_fault epb cat_l3 cdp_l3 invpcid_single intel_ppin ssbd mba ibrs ibpb stibp i brs_enhanced tpr_shadow vnmi flexpriority ept vpid fsqsbase tsc_adjust bmi1 hle avx2 smep bmi2 erms invpcid rtm cqm mpq rdt_a avx512f avx512dq rdseed adx smap clflushopt clwb intel_pt avx512cd avx512bw avx512vl xsaveopt xsavec xgetbv1 xsaves cqmq_llc cqmq_occup_llc cqmq_mb m_total cqmq_mb_local dtherm ida arat pln pts pku ospke avx512_vnni md_clear flush_l1d arc_h_capabilities
```

[9]: `# Check to see if system is GPU:  
!nvidia-smi`

```
Fri Feb 18 00:15:50 2022
```

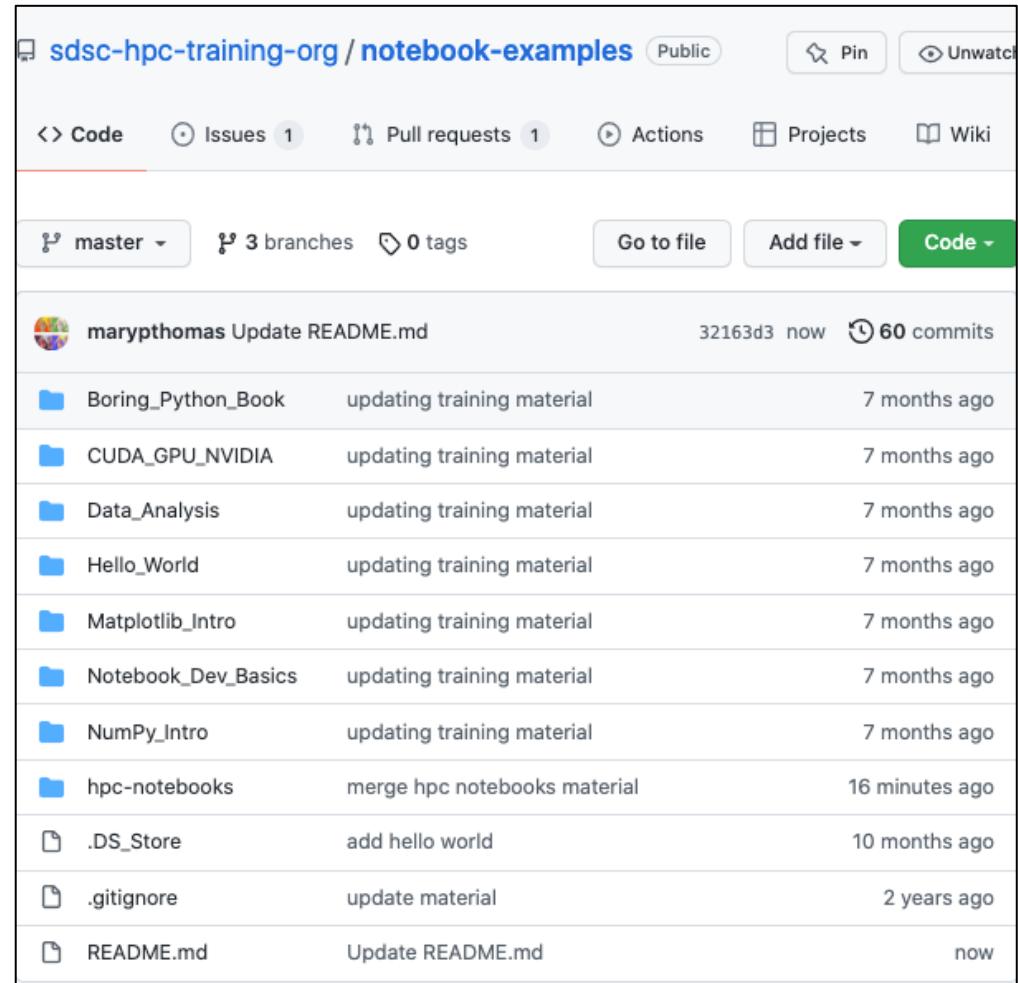
NVIDIA-SMI 460.32.03		Driver Version: 460.32.03		CUDA Version: 11.2	
GPU Name	Persistence-M	Bus Id	Disp.A	Volatile	Uncorr. ECC
Fan	Temp	Perf	Pwr:Usage/Cap	Memory-Usage	GPU-Util Compute M.
					MIG M.
0 Tesla V100-SXM2...	On	00000000:18:00.0	Off	0%	Default
N/A 37C	P0	68W / 300W	0MiB / 32510MiB		N/A

[10]: `# if you see: /bin/bash: nvidia-smi: command not found  
# the system is not GPU`

# 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



The screenshot shows the GitHub repository page for "sdsc-hpc-training-org / notebook-examples". The repository is public, as indicated by the button at the top right. The main navigation tabs are "Code", "Issues (1)", "Pull requests (1)", "Actions", "Projects", and "Wiki". Below these, there are buttons for "master", "3 branches", "0 tags", "Go to file", "Add file", and "Code". The commit history is listed below, showing 60 commits from "marypthomas" and others, all related to updating training material. The commits are dated from "now" to "16 minutes ago".

Commit	Message	Date
marypthomas	Update README.md	32163d3 now 60 commits
Boring_Python_Book	updating training material	7 months ago
CUDA_GPU_NVIDIA	updating training material	7 months ago
Data_Analysis	updating training material	7 months ago
Hello_World	updating training material	7 months ago
Matplotlib_Intro	updating training material	7 months ago
Notebook_Dev_Basics	updating training material	7 months ago
NumPy_Intro	updating training material	7 months ago
hpc-notebooks	merge hpc notebooks material	16 minutes ago
.DS_Store	add hello world	10 months ago
.gitignore	update material	2 years ago
README.md	Update README.md	now

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  - High-performance computing (HPC)
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- Interactive Application Examples
  - Viewing Data: unix file ops (grep, awk, cat), gnuplot, NetCDF
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- Q&A

# Expanse User Portal

**SIMPLIFY!  
EXPANSE PORTAL**

The portal provides an integrated, and easy to use interface to access Expanse HPC resources.

With the portal, researchers can manage files (create, edit, move, upload, and download), view job templates for various applications, submit and monitor jobs, run interactive applications, and connect via SSH. The portal has no end-user installation requirements other than access to a modern up-to-date web browser.

**Pinned Apps A featured subset of all available apps**

- Action Jobs
- Home Directory
- Job Composer
- Expanse Shell Access
- MATLAB
- RSTUDIO
- Allocation and Usage Information
- Jupyter

**Active Jobs**

**OOD 2.0 Features**

**Interactive Services**

**Job Script Editing and Submission**

**Active Job monitoring and Management**

- <https://portal.expanse.sdsc.edu>; authenticate using ACCESS credentials
- Securely hosts batch job submission & monitoring, and interactive applications
- Simplifies launching supported interactive applications → manages software dependencies

# Expanse Portal: File Management

The image shows the Expanse Portal interface. At the top, there is a toolbar with buttons for 'Open in Terminal' (circled in red), 'New File', 'New Directory', 'Upload', 'Download', and 'Copy/Mov'. Below the toolbar is a breadcrumb navigation bar showing the path: '/ home / mthomas / expanse /' and a 'Change directory' button. There are also checkboxes for 'Show Owner/Mode', 'Show Dotfiles', and a 'Filter' input field. A message indicates 'Showing 28 of 62 rows'. The main area is a table listing files and directories:

Type	Name	Size	Modified at
Folder	classes	-	4/15/2022 3:37:19 PM
Folder	comet-files	-	2/16/2022 6:41:00 PM
Folder	conda-install-tmp	-	10/29/2020 2:27:20 AM
Folder	dev	-	2/16/2022 8:39:49 PM
Folder	galileo-examples	-	7/27/2022 2:27:08 AM
Folder	galileo-repo	-	2/16/2022 6:36:21 PM
Folder	gnuplot-ex	-	8/1/2022 8:50:45 PM
Folder	gpuhack22	-	5/11/2022 3:40:13 PM
Folder	hpctr-examples	-	6/27/2022 1:31:14 PM
Folder	hptrain	-	2/16/2022 8:47:23 PM

A red arrow points from the 'Open in Terminal' button in the toolbar to a terminal window on the right side of the interface. The terminal window shows a session on host 'login.expanse.sdsc.edu' with the initial directory '/home/mthomas/expanse'. The session lists numerous files and their details, such as owner, size, and modification date. The terminal prompt is '[mthomas@login01 ~]\$'.

```
mpt@SDSC: ~ % portal.expanse.sdsc.edu/pun/sys/shell/ssh/default/home/mthomas/expanse
Host: login.expanse.sdsc.edu  Initial directory: /home/mthomas/expanse
-rw----- 1 mthomas use300 17803 Aug 1 21:33 .viminfo
-rw-r--r-- 1 mthomas use300 36 Jan 27 2022 .vimrc
drwxr--r-- 2 mthomas use300 4 Aug 1 23:11 .vnc
-rw-r--r-- 1 mthomas use300 173 Oct 7 2020 .wget-hsts
-rw-r--r-- 1 mthomas use300 124 Oct 7 2020 README.txt
drwxr-xr-x 4 mthomas use300 4 Apr 15 15:37 classes
drwxr-xr-x 2 mthomas use300 6 Feb 16 18:41 comet-files
-rw-r--r-- 1 mthomas use300 116 Mar 4 2021 conda-activate.txt
drwxr-xr-x 2 mthomas use300 4 Oct 29 2020 conda-install-tmp
drwxr-xr-x 8 mthomas use300 8 Feb 16 20:39 dev
-rw-r--r-- 1 mthomas use300 12266 Nov 8 2021 ex.cl.cmds
drwxr-xr-x 3 mthomas use300 8 Jul 27 02:27 galileo-examples
drwxr-xr-x 5 mthomas use300 9 Feb 16 18:36 galileo-repo
drwxr-xr-x 2 mthomas use300 10 Aug 1 20:50 gnuplot-ex
drwxr-xr-x 3 mthomas use300 3 May 11 15:40 gpuhack22
drwxr-xr-x 13 mthomas use300 16 Jun 27 13:31 hpctr-examples
drwxr-xr-x 5 mthomas use300 6 Feb 16 20:47 hpctrain
drwxr-xr-x 2 mthomas use300 8 Jul 27 02:33 interactive.ex
drwxr-xr-x 2 mthomas use300 3 Aug 1 21:33 matlab-ex
drwxr-xr-x 24 mthomas use300 27 Jul 27 2021 miniconda3
drwxr-xr-x 3 mthomas use300 5 Jul 27 2021 ml-dev-mary
-rwx----- 1 mthomas use300 235 Jun 1 2021 modules.cpu.txt
-rwx----- 1 mthomas use300 84 Feb 8 2021 modules.gpu.txt
-rw-r--r-- 1 mthomas use300 6178 Mar 4 2021 modules.marty.ex.txt
drwxr-xr-x 3 mthomas use300 4 Jul 18 16:09 nn-pde-TEST
drwxr-xr-x 10 mthomas use300 13 Jul 28 2021 notebook-examples
drwxr-xr-x 22 mthomas use300 26 Jul 20 2021 notebook-examples-dev
-rwxr-xr-x 1 mthomas use300 234277552 Aug 1 20:04 ocean_his.nc.gz
drwxr-xr-x 9 mthomas use300 19 Jul 28 2021 reverse-proxy
drwxr-xr-x 2 mthomas use300 7 Feb 16 18:44 scc21
drwxr-xr-x 2 mthomas use300 5 Feb 16 20:37 tensorflow
drwxr-xr-x 2 mthomas use300 3 Jul 14 2021 tools
[mthomas@login01 ~]$
```

# Expanse Portal: Running Matlab

The image shows a multi-step process for launching a Matlab session on the Expanse Portal.

**Step 1: Interactive Apps Selection**

The user selects "MATLAB" from the "Interactive Apps" list. A tooltip provides instructions: "This app will launch a MATLAB GUI on Expanse. You will be able to interact with the MATLAB GUI through a VNC session. Please email help@xsede.org to be added to matlab-groups." The "Session ID" is listed as "fee7f0fb-48df-46af-814".

**Step 2: Session Configuration**

The user fills out the following configuration fields:

- Partition:** compute
- Reservation:** (empty)
- Number of hours:** 1
- Account:** use300
- Checkboxes:** "I would like to receive an email when the session starts" (checked) and "Working directory" (set to "home")
- Number of cores:** 1
- Memory (GB):** 64

**Step 3: Session Launch**

The user clicks the "Launch" button. A success message appears: "Session was successfully deleted."

**Step 4: Session Overview**

The user views the session details:

- Host:** >\_exp-1-18-expance.sdsc.edu
- Created at:** 2022-08-01 22:48:55 PDT
- Time Remaining:** (not shown)
- Session ID:** 14834793
- Nodes:** 1 node | **Cores:** 128 cores | **Status:** Running

**Step 5: Matlab Session View**

The user launches the Matlab session. The Matlab interface shows:

- Current Folder:** /home/mthomas
- Command Window:** (partial logs)

```
>> plot sin(22)
Error using plot
Invalid first data argument.

>> x = 0:pi/100:2*pi;
>> y = sin(x);
>> plot(x,y)
Warning: MATLAB has disabled some advanced rendering features by switching to software rendering. For more information, click here.
f2 >
```
- Figure 1:** A plot of the sine function from 0 to 2π.

# Expanse Portal: Launching Notebooks

The screenshot illustrates the Expanse Portal's Jupyter Session feature. It consists of three main components:

- Left Panel (Top):** A "Jupyter Session" configuration form. Fields include:
  - Account: use300
  - Partition (Please choose the gpu, gpu-shared, or gpu-preempt as the partition if using gpus): shared
  - Time limit (min): 30
  - Number of cores: 1
  - Memory required per node (GB): 2
  - GPUs (optional): 0
- Middle Panel:** A file browser window showing files in the directory `/notebook-examples /Hello_World /`. The files listed are:
  - hello\_world.ipynb (selected)
  - hello.py
  - README.md
- Right Panel:** A Jupyter Notebook interface with two tabs open:
  - `numpy_intro.ipynb`: Contains code related to memory management and system monitoring.
  - `hello_world_gpu.ipynb`: Contains code to check for GPU availability using `nvidia-smi`. The output shows an error message: "NVIDIA-SMI has failed because it couldn't communicate with the NVIDIA driver. Make sure that the latest NVIDIA driver is installed and running."

# Expanse Portal: Input data example for Jupyter Notebook

**Account:** use300

**Partition:** (Please choose the gpu, gpu-shared, or gpu-preempt as the partition if using gpus): debug

**Time limit (min):** 30

**Number of cores:** 1

**Memory required per node (GB):** 2

**GPUs (optional):** 0

**Singularity Image File Location:** (Use your own or to include from existing container library at /cm/shared/apps/container e.g.,

/cm/shared/apps/containers/singularity/pytorch/pytorch-latest.sif)

/cm/shared/apps/containers/singularity/pytorch/pytorch-latest.sif

**Environment modules to be loaded** (E.g., to use latest version of system Anaconda3 include cpu,gcc,anaconda3): singularitypro

**Conda Environment** (Enter your own conda environment if any):

**Conda Init** (Provide path to conda initialization scripts):

**Conda Yaml** (Upload a yaml file to build the conda environment at runtime) No file chosen:

**Turn on use of mamba for speeding up conda-yml installs:**

**Enable use of new caching mechanism that will store and reuse conda-yml created environments using conda-pack !????**

**Reservation:**

**QoS:**

**Working directory:** HOME

**Type:** JupyterLab

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# Thank You!

## Q&A

If you have problems, please contact **consult@sdsc.edu**

<https://github.com/sdsc-complecs/interactive-computing/>

# Resources

- GitHub Repo for this presentation:
  - <https://github.com/sdsc-complecs/interactive-computing/>
- SDSC Training Resources
  - [https://www.sdsc.edu/education\\_and\\_training/training](https://www.sdsc.edu/education_and_training/training)
  - <https://github.com/sdsc-hpc-training-org/notebook-examples>
  - <https://github.com/mkandes/galyleo>
- Expanse :
  - Landing page: [expanse.sdsc.edu](https://expanse.sdsc.edu)
  - User Guide: [https://expanse.sdsc.edu/support/user\\_guides/expanse.html](https://expanse.sdsc.edu/support/user_guides/expanse.html)
  - Training: [https://www.sdsc.edu/education\\_and\\_training/training\\_hpc.html](https://www.sdsc.edu/education_and_training/training_hpc.html)
- Problems? Contact [consult@sdsc.edu](mailto:consult@sdsc.edu)