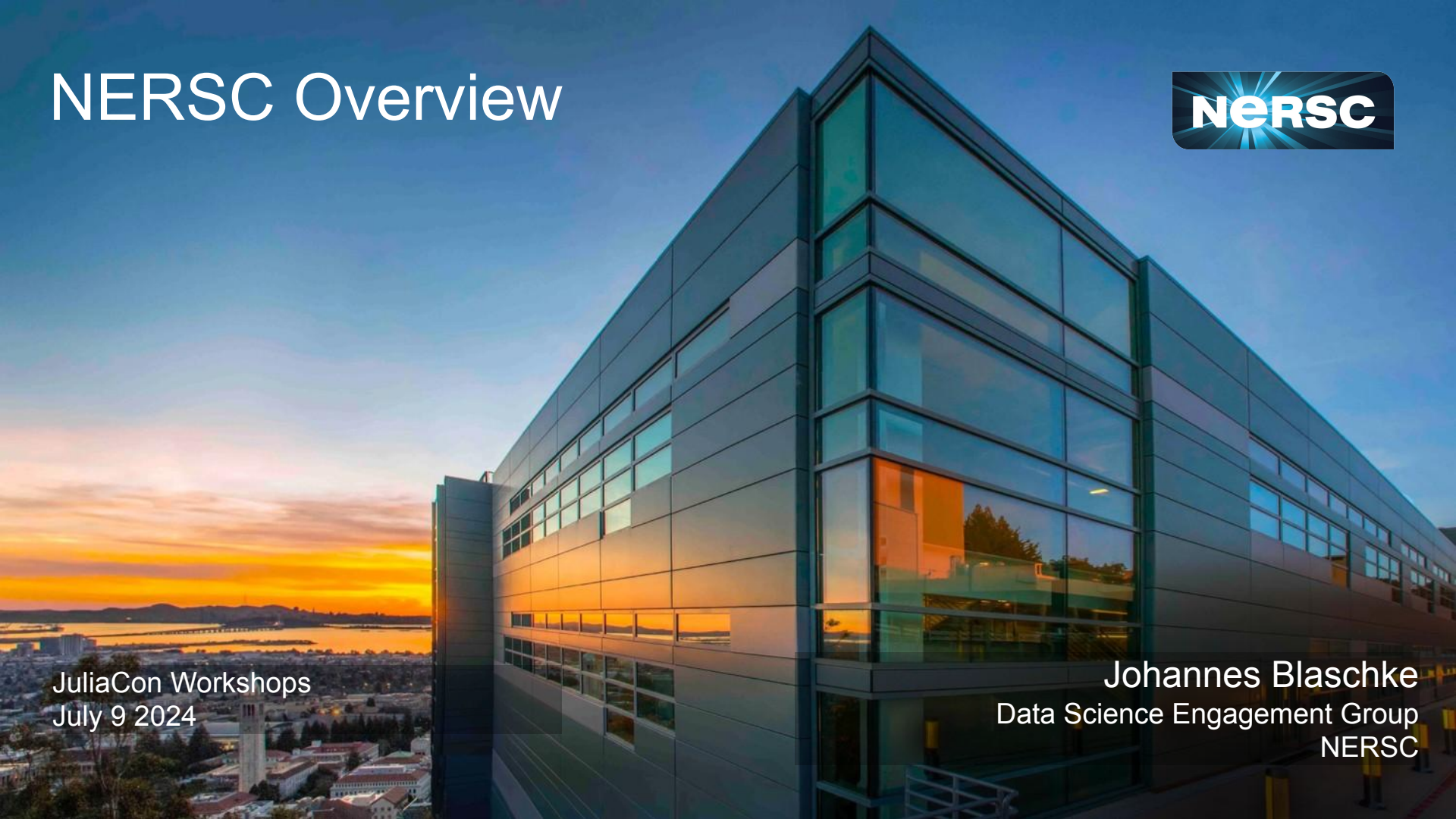
NERSC Overview



JuliaCon Workshops
July 9 2024

Johannes Blaschke
Data Science Engagement Group
NERSC

National Energy Research Scientific Computing Center

- NERSC is a national supercomputer center funded by the U.S. Department of Energy Office of Science (SC)
  - Supports SC research mission
  - Part of Berkeley Lab
- Researchers with funding from SC who need supercomputing resources can use NERSC
  - Other researchers can apply if research is in SC mission
- NERSC supports 10,000 users, 1,000 projects
  - From all 50 states + international; 60% from universities
  - Hundreds of users log on each day

NERSC User Demographics

~10,000 Annual Users from ~800 Institutions + National Labs

32% Graduate Students

19% Postdoctoral Fellows

15% Staff Scientists

13% University Faculty

8% Undergraduate Students

5% Professional Staff

60% Universities

29% DOE Labs

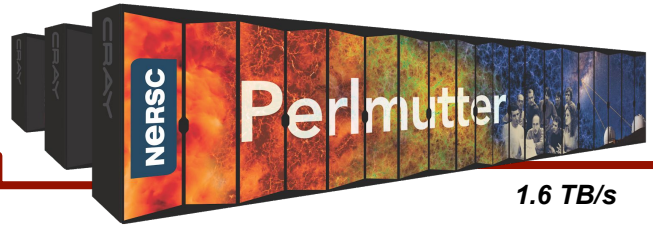
5% Other Government Labs

4% Industry

1% Small Businesses

<1% Private Labs

NERSC Systems Ecosystem



TOP 500 The List.
#8, 93.8PF Peak

>5 *TB/s*

35 PB All-Flash Scratch

HPE Slingshot 11 interconnect
4 NICs/GPU node,
1 NIC/CPU node

1.6 TB/s

1,792 GPU-accelerated nodes
4 NVIDIA A100 GPUs+1 AMD "Milan" CPU
448 TB (CPU) + 320 TB (GPU) memory

3,072 CPU-only nodes
2 AMD "Milan" CPUs
1,536 TB CPU memory

Off-Platform Storage

50 GB/s — HPSS Tape Archive ~300 PB

100 GB/s — Common File System 130 PB

5 GB/s — /home 450 TB

DTNs, Gateways

Spin edge services

Ethernet
Science Friendly Security
Production Monitoring
Power Efficiency
LAN

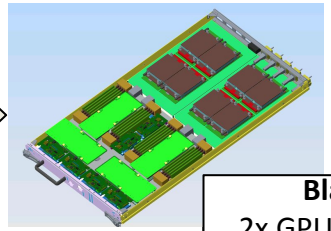
ESnet ENERGY SCIENCES NETWORK
2 x 400 Gb/s
2 x 100 Gb/s

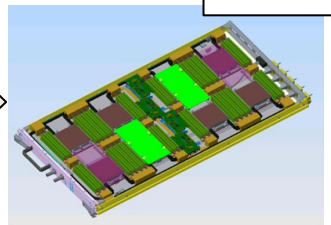
Experimental Facility | ASCR Facility | Home Institution | Cloud | Edge

Perlmutter system configuration

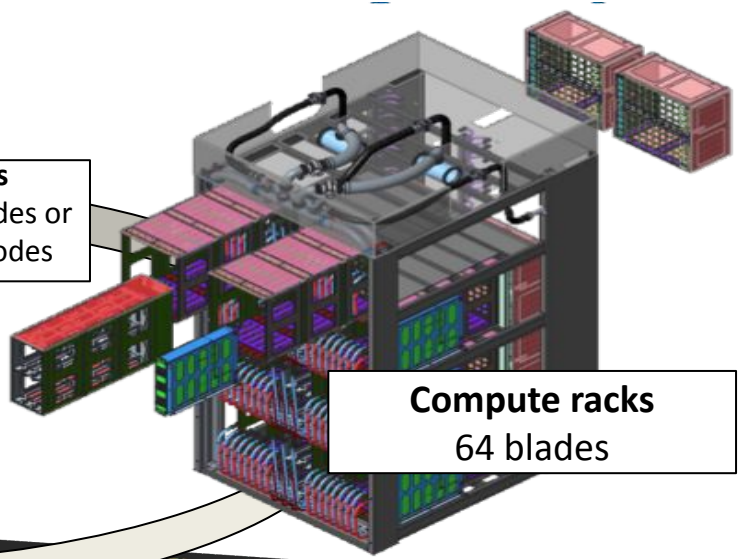
NVIDIA "Ampere" GPU Nodes
4x GPU + 1x CPU
40 GiB HBM + 256 GiB DDR
4x 200G "Slingshot" NICs

AMD "Milan" CPU Node
2x CPUs
> 256 GiB DDR4
1x 200G "Slingshot" NIC





Blades
2x GPU nodes or
4x CPU nodes

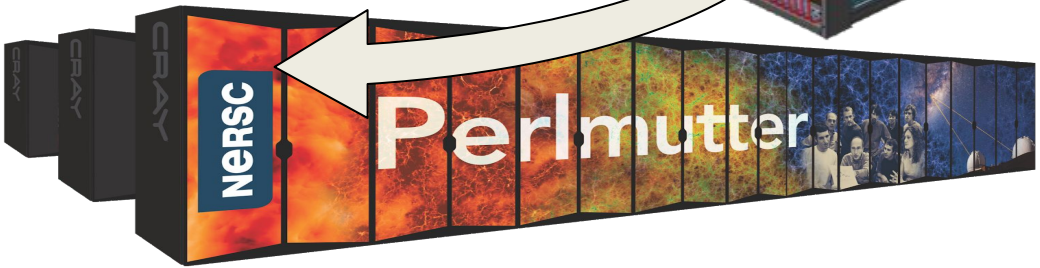


Compute racks
64 blades

Centers of Excellence
Network
Storage
App. Readiness
System SW

→

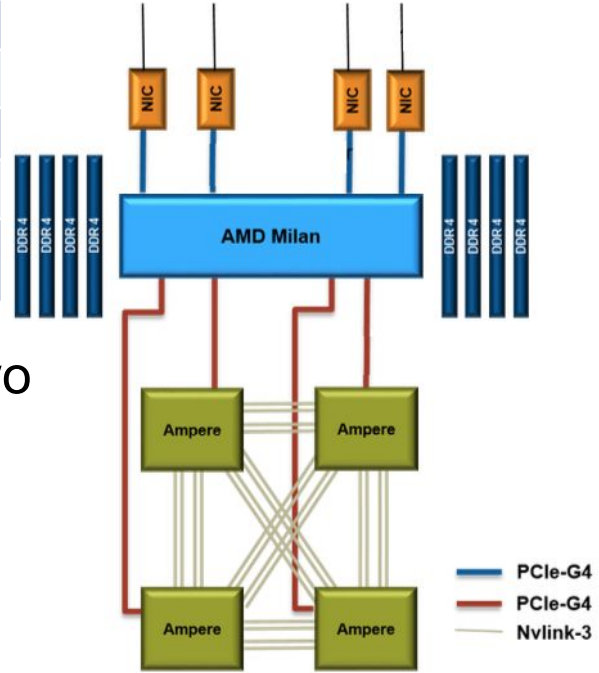
Perlmutter system
GPU racks
CPU racks
~6 MW



Node Types

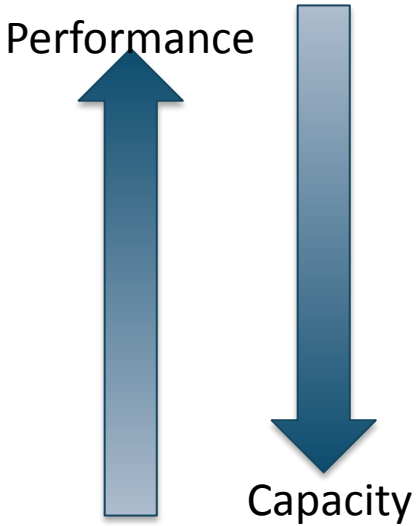
Partition	Nodes	CPU	RAM	GPU	NIC
GPU	1536	1x AMD EPYC 7763	256GB	4x NVIDIA A100 (40GB)	4x HPE Slingshot 11
	256	1x AMD EPYC 7763	256GB	4x NVIDIA A100 (80GB)	4x HPE Slingshot 11
CPU	3072	2x AMD EPYC 7763	512GB	–	1x HPE Slingshot 11
Login	40	1x AMD EPYC 7713	512GB	4x NVIDIA A100 (40GB)	–
Large Memory	4	1x AMD EPYC 7713	1TB	4x NVIDIA A100 (40GB)	1x HPE Slingshot 11

GPU Node Architecture:



- Each Milan CPU has 64 2.45 GHz cores with two hardware threads
- Access is managed via Slurm partitions
- Login nodes are GPU-enabled

Simplified NERSC File Systems



Memory

Burst Buffer

Scratch

Community

HPSS

Global Common

Global Home

35 PB Flash Scratch
Lustre >5 TB/s
temporarily (purge)
xGB (x=Total RAM) In-Memory Burst Buffer
/tmp RamFS
157 PB HDD Community
Spectrum Scale (GPFS)
150 GB/s, permanent
150 PB Tape Archive
HPSS Forever
20 TB SSD Software
Spectrum Scale
Permanent
Faster compiling / Source Code

Global File Systems

Global Home

- Permanent, relatively small storage
- Mounted on all platforms
- NOT tuned to perform well for parallel jobs
- Quota cannot be changed
- Snapshot backups (7-day history)
- **Perfect for storing data such as source code, shell scripts**
- **Addressed using `$HOME`**

Community File System (CFS)

- Permanent, larger storage
- Mounted on all platforms
- Medium performance for parallel jobs
- Quota can be changed
- Snapshot backups (7-day history)
- **Perfect for sharing data within research group**
- **Addressed using `$CFS`**

Local File Systems

Scratch

- Large, temporary storage
- Optimized for read/write operations, NOT storage
- Not backed up
- Purge policy (8 weeks)
- **Perfect for staging data and performing computations**
- **Addressed using `$SCRATCH`**

Burst Buffer

- Temporary storage
- High-performance in-memory file system
- **Perfect for getting good performance in I/O-constrained codes**
- Not shared between nodes

There are many different ways to access NERSC. To use our resources, you need to either:

1. Log into the login nodes and interact with Slurm (covered here)
2. Use services (eg. Jupyter) that expose web interfaces (covered later)
3. Interact via our REST API – called the “Superfacility API” (covered later)

Connecting with SSH

- To access Perlmutter, use:
  `saul-p1.nersc.gov`
  `perlmutter-p1.nersc.gov`

```
blaschke@laptop:~$ ssh <user>@saul-p1.nersc.gov
blaschke@laptop:~$ ssh <user>@perlmutter-p1.nersc.gov
```

- To be able to open GUI applications on the login nodes use: `ssh -Y`

```
blaschke@laptop:~$ ssh -Y <user>@saul-p1.nersc.gov
```

Connecting with SSH

After successfully logging on, you be greeted by the terms of use, and the command-line input prompt:

```
For past outages, see: https://my.nersc.gov/outagelog-cs.p
blaschke@perlmutter:login17:↝
```

From here you can interact with perlmutter…

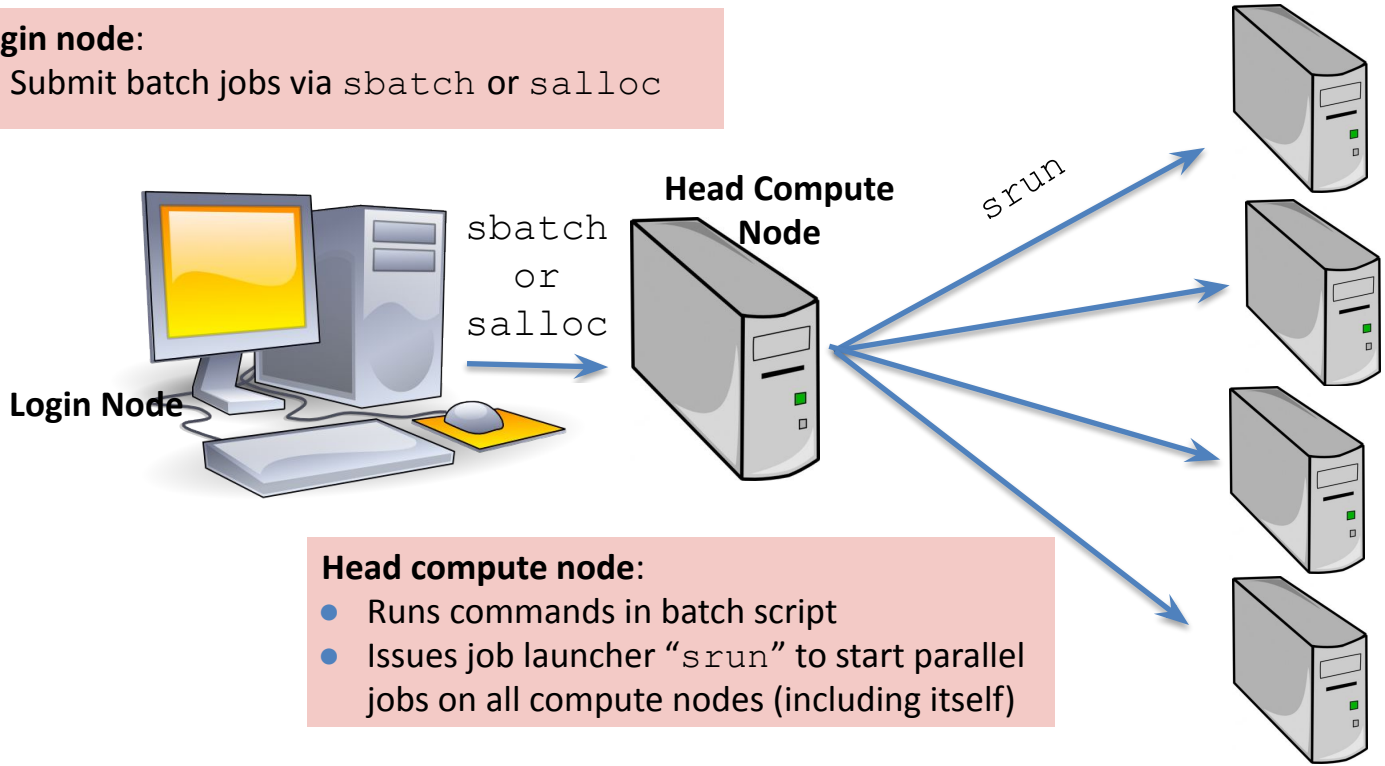
```
blaschke@laptop:~$ ssh blaschke@saul-p1.nersc.gov
********************************************************************************
                        NOTICE TO USERS

Lawrence Berkeley National Laboratory operates this computer system under
contract to the U.S. Department of Energy.  This computer system is the
property of the United States Government and is for authorized use only.
Users (authorized or unauthorized) have no explicit or implicit
expectation of privacy.

Any or all uses of this system and all files on this system may be
intercepted, monitored, recorded, copied, audited, inspected, and disclosed
to authorized site, Department of Energy, and law enforcement personnel,
as well as authorized officials of other agencies, both domestic and foreign.
By using this system, the user consents to such interception, monitoring,
recording, copying, auditing, inspection, and disclosure at the discretion
of authorized site or Department of Energy personnel.

Unauthorized or improper use of this system may result in administrative
disciplinary action and civil and criminal penalties. By continuing to use
this system you indicate your awareness of and consent to these terms and
conditions of use. LOG OFF IMMEDIATELY if you do not agree to the conditions
stated in this warning.

********************************************************************************

Login connection to host x3114c0s15b0n0:


################################################################################
              _                  _   _
             | |                | | | |
 _ __   ___ _ __| |_ _ __ ___   _| |_| |_ ___ _ __
| '_ \ / _ \ '__| | '_ ` _ \| | | __| __/ _ \ '__|
| |_) |  __/ |  | | | | | | | |_| | |_| ||  __/ |
| .__/ \___|_|  |_|_| |_| |_|\__,_|\__|\__\___|_|
| |
|_|

Hello, World!

Welcome to perlmutter!
################################################################################

For all planned outages, see: https://www.nersc.gov/live-status/motd/

For past outages, see: https://my.nersc.gov/outagelog-cs.p p/
blaschke@perlmutter:login17:↝
```

Submitting Jobs

- Jobs can be submitted to queueing system through sbatch or salloc:
  - `sbatch <my_job_script>`
  - `salloc <options>`
- The above methods list details about resources needed for a job and for how long
- Eg.: a request for a cpu node to be allocated for 5 mins:
  - `salloc -N 1 -C cpu -q debug -t 5 -A <project>`

Submitting Jobs

Login node:
- Submit batch jobs via `sbatch` or `salloc`



Head compute node:
- Runs commands in batch script
- Issues job launcher "`srun`" to start parallel jobs on all compute nodes (including itself)

*figure courtesy Helen (2020 NERSC Training)

My First “Hello World” Job Script

debug queue

2 nodes

10 min “walltime”

run on haswell partition

use SCRATCH file system

my_batch_script.sh

```
#!/bin/bash
#SBATCH -q debug
#SBATCH -N 2
#SBATCH -t 10:00
#SBATCH -C haswell
#SBATCH -L SCRATCH
#SBATCH -J myjob
srun -n 64 ./helloWorld
```

To run via batch queue

```
% sbatch my_batch_script.sh
```

To run via interactive batch

```
% salloc -N 2 -q interactive -C haswell -t 10:00
```

<wait_for_session_prompt. Land on a compute node>

```
% srun -n 64 ./helloWorld
```

Anatomy of a Batch Script

my_batch_script.sh

```
#!/bin/bash
#SBATCH --account=mxxx
#SBATCH --qos=regular
#SBATCH --nodes=2
#SBATCH --time=60
#SBATCH --constraint=gpu
#SBATCH --jobname=myjob
#SBATCH --license=scratch,cfs

export OMP_NUM_THREADS=1
srun -n 64 <executable>
```

my_batch_script.sh

```
#!/bin/bash
#SBATCH -A mxxx
#SBATCH -q regular
#SBATCH -N 2
#SBATCH -t 12:00:00
#SBATCH -C gpu
#SBATCH -J myjob
#SBATCH -L scratch,cfs

export OMP_NUM_THREADS=1
srun -n 64 <executable>
```

Anatomy of a Batch Script

`#!` – Job scripts are bash scripts

my_batch_script.sh

```
#!/bin/bash
#SBATCH --account=mxxx
#SBATCH --qos=regular
#SBATCH --nodes=2
#SBATCH --time=60
#SBATCH --constraint=gpu
#SBATCH --jobname=myjob
#SBATCH --license=scratch,cfs

export OMP_NUM_THREADS=1
srun -n 64 <executable>
```

my_batch_script.sh

```
#!/bin/bash
#SBATCH -A mxxx
#SBATCH -q regular
#SBATCH -N 2
#SBATCH -t 12:00:00
#SBATCH -C gpu
#SBATCH -J myjob
#SBATCH -L scratch,cfs

export OMP_NUM_THREADS=1
srun -n 64 <executable>
```

Anatomy of a Batch Script

Preamble. All flags after `#SBATCH` are passed to slurm

my_batch_script.sh

```
#!/bin/bash
#SBATCH --account=mxxx
#SBATCH --qos=regular
#SBATCH --nodes=2
#SBATCH --time=60
#SBATCH --constraint=gpu
#SBATCH --jobname=myjob
#SBATCH --license=scratch,cfs

export OMP_NUM_THREADS=1
srun -n 64 <executable>
```

my_batch_script.sh

```
#!/bin/bash
#SBATCH -A mxxx
#SBATCH -q regular
#SBATCH -N 2
#SBATCH -t 12:00:00
#SBATCH -C gpu
#SBATCH -J myjob
#SBATCH -L scratch,cfs

export OMP_NUM_THREADS=1
srun -n 64 <executable>
```

Anatomy of a Batch Script

Setup. Environment variables control many aspects of HPC libraries.

my_batch_script.sh

```
#!/bin/bash
#SBATCH --account=mxxx
#SBATCH --qos=regular
#SBATCH --nodes=2
#SBATCH --time=60
#SBATCH --constraint=gpu
#SBATCH --jobname=myjob
#SBATCH --license=scratch,cfs

export OMP_NUM_THREADS=1
srun -n 64 <executable>
```

my_batch_script.sh

```
#!/bin/bash
#SBATCH -A mxxx
#SBATCH -q regular
#SBATCH -N 2
#SBATCH -t 12:00:00
#SBATCH -C gpu
#SBATCH -J myjob
#SBATCH -L scratch,cfs

export OMP_NUM_THREADS=1
srun -n 64 <executable>
```

Anatomy of a Batch Script

`srun` launches the executable on all nodes (and provides MPI)

my_batch_script.sh

```
#!/bin/bash
#SBATCH --account=mxxx
#SBATCH --qos=regular
#SBATCH --nodes=2
#SBATCH --time=60
#SBATCH --constraint=gpu
#SBATCH --jobname=myjob
#SBATCH --license=scratch,cfs

export OMP_NUM_THREADS=1
srun -n 64 <executable>
```

my_batch_script.sh

```
#!/bin/bash
#SBATCH -A mxxx
#SBATCH -q regular
#SBATCH -N 2
#SBATCH -t 12:00:00
#SBATCH -C gpu
#SBATCH -J myjob
#SBATCH -L scratch,cfs

export OMP_NUM_THREADS=1
srun -n 64 <executable>
```

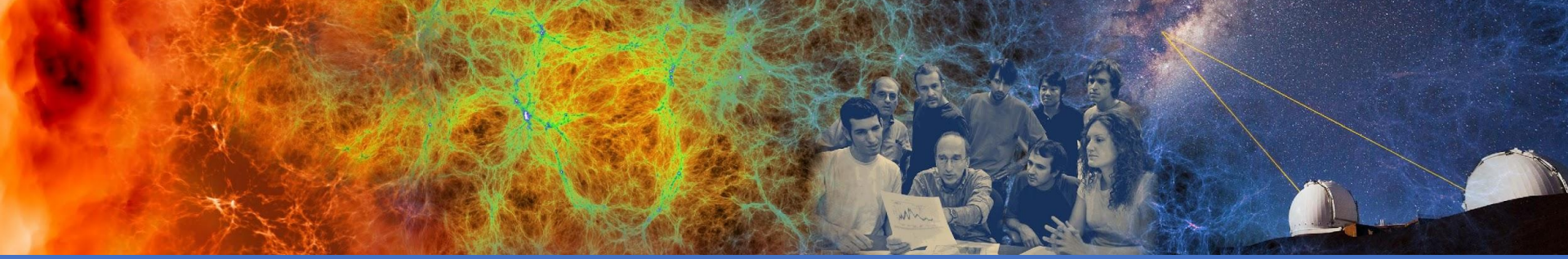
Sample Batch Script for a GPU node

gpu_node.sh

```
#!/bin/bash
#SBATCH --account=mxxx
#SBATCH --qos=regular
#SBATCH --nodes=2
#SBATCH --time=60
#SBATCH --constraint=gpu
#SBATCH --jobname=myjob
#SBATCH --ntasks-per-node=64
#SBATCH --cpus-per-task=2
#SBATCH --gpus-per-node=4

export OMP_NUM_THREADS=1
srun -n 128 <executable>
```

c = 2*(64/k)

where:
k = ntasks-per-node



NERSC Training Accounts

for *Hands-on with Julia for HPC on GPUs and CPUs*

NERSC

BERKELEY LAB

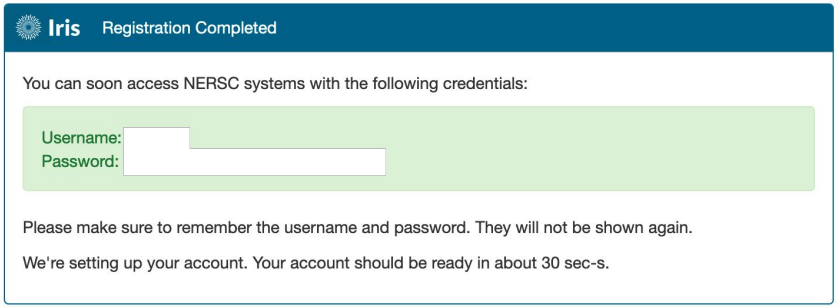
U.S. DEPARTMENT OF ENERGY | Office of Science

Activate your Training Account

- Go to: https://iris.nersc.gov/train

- Enter the Training Code: “enxl” along with your details
  Note: if you have previously registered an account using a different code please recreate it.

- **Important: make a copy of your login and password** you won’t be able to change these, nor recover them later!!!



Access to Perlmutter and Use Julia Module

- NERSC users have been added to ntrain9 project
- Non-users were sent the instruction to get a training account
  - Account valid through July 14
- Login to Perlmutter: ssh username@perlmutter.nersc.gov
- Julia modules:
  - `% module use /global/common/software/nersc/n9/julia/modules`
  - `% module load PrgEnv-gnu`
  - `% module load julia`
- Running Jobs examples:
  - https://docs.nersc.gov/jobs/

Compute Node Reservations

- GPU node reservation: 1pm - 4pm EDT, Tues June 18
  - To use 1 GPU only (sample flags for `sbatch` or `salloc`):
    - `-A ntrain1 --reservation=julia_training -C gpu -N 1 -c 32 -G 1 -t 30:00 -q shared`
  - To use multiple nodes (sample flags for sbatch or salloc):
    - `-A ntrain1 --reservation=julia_training -C gpu -N 2 -t 30:00 -q regular`
- Outside of reservation, use:
  - To use 1 GPU only (sample flags for sbatch or salloc):
    - `-A <project> -C gpu -N 1 -c 32 -G 1 -t 30:00 -q shared`
  - To use multiple nodes (sample flags for sbatch or salloc):
    - `-A <project> -C gpu -N 2 -t 30:00 -q regular` (or `-q interactive` for salloc)

Reminder about file Systems

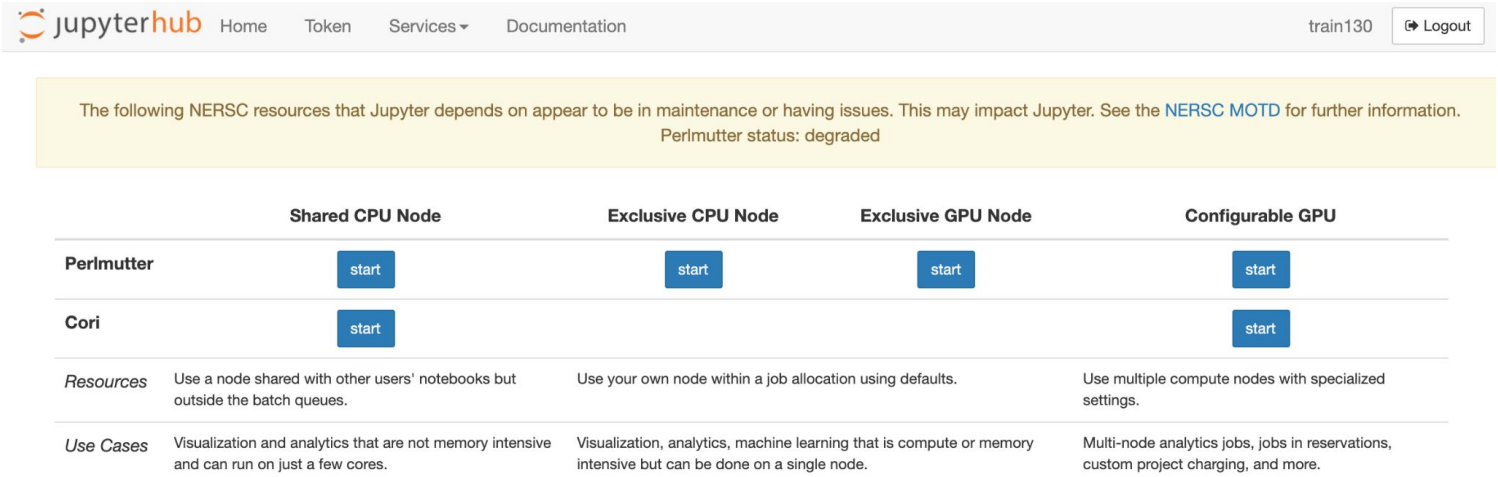
`$HOME` is not the best file system for running jobs at scale. Consider therefore replacing all occurrences of `$HOME` with `$SCRATCH` in the NERSC scripts here:

https://github.com/JuliaHPC/juliacon24-hpcworkshop.git

Pro tip: add `export JULIA_DEPOT_PATH=$SCRATCH/depot` to you scripts for optimal performance (remember to do this in the config script, **and** the job scrip)

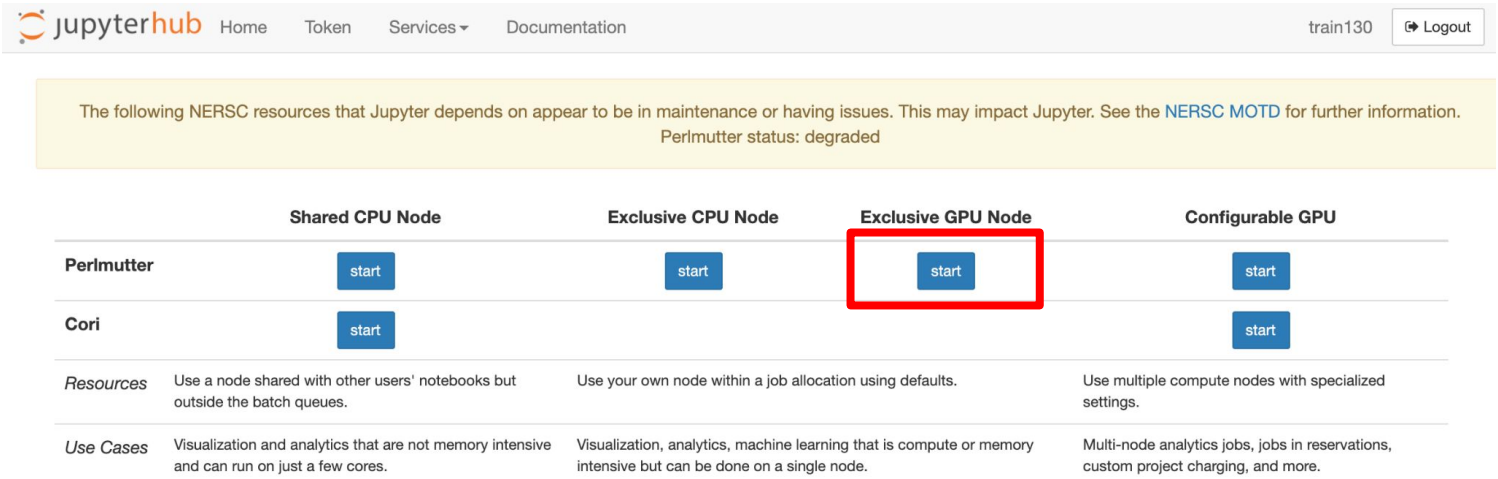
Logging into Jupyter

- Go to https://jupyter.nersc.gov
- Sign in using your training account credentials
- Select your preferred jupyter instance:



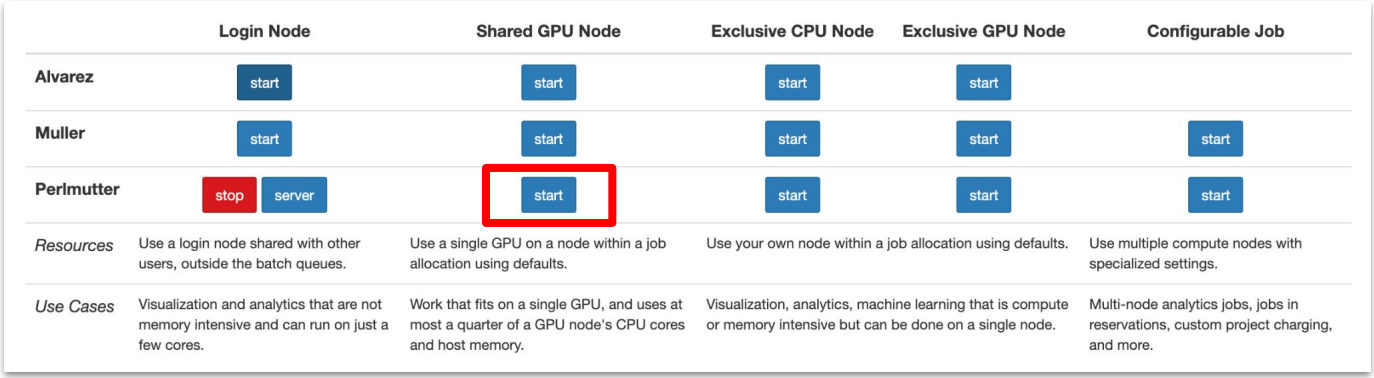
Setup

- Go to https://jupyter.nersc.gov and select: "Exclusive GPU Node" in the "Perlmutter" row



Setup

If you're spending a long time in the queue waiting for an exclusive GPU node, "Shared GPU Node"s are also available – eg:

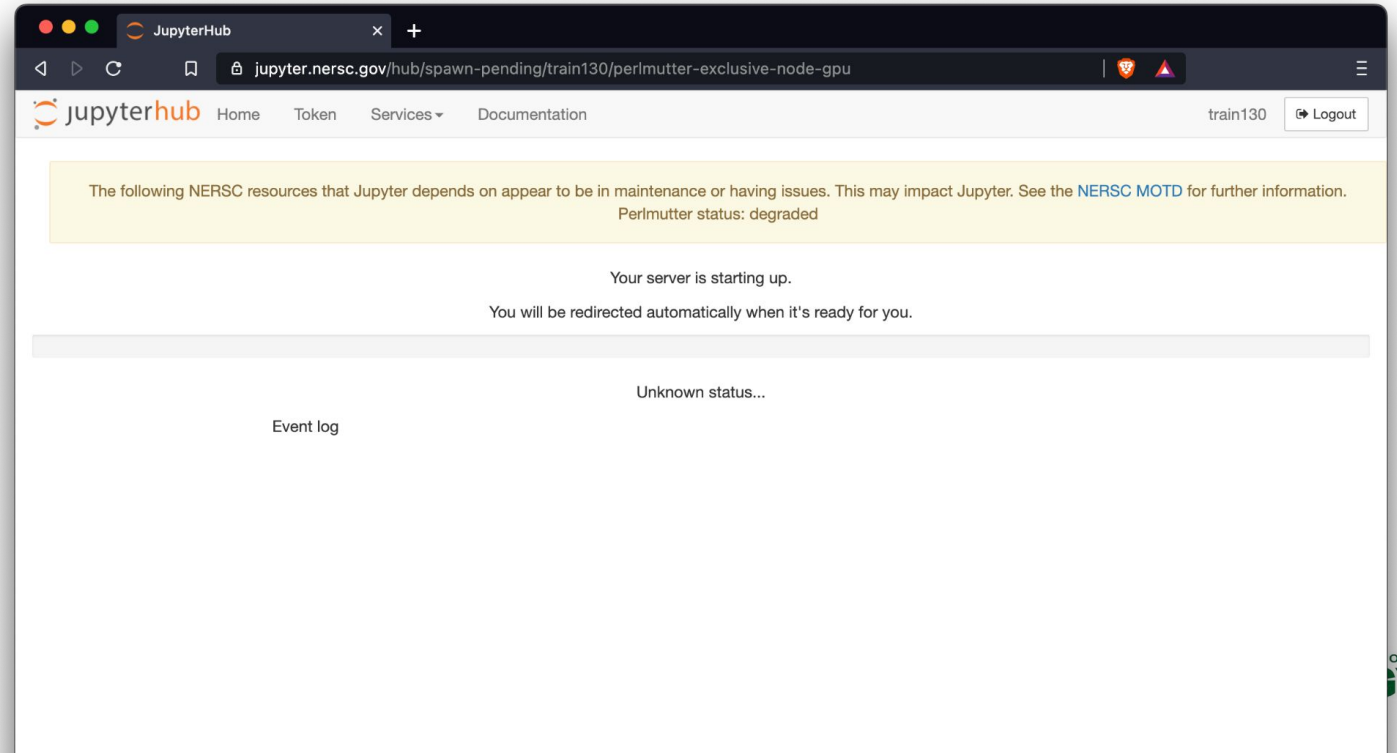


	Login Node	Shared GPU Node	Exclusive CPU Node	Exclusive GPU Node	Configurable Job
Alvarez	start	start	start	start	
Muller	start	start	start	start	start
Perlmutter	stop server	start	start	start	start
Resources	Use a login node shared with other users, outside the batch queues.	Use a single GPU on a node within a job allocation using defaults.	Use your own node within a job allocation using defaults.		Use multiple compute nodes with specialized settings.
Use Cases	Visualization and analytics that are not memory intensive and can run on just a few cores.	Work that fits on a single GPU, and uses at most a quarter of a GPU node's CPU cores and host memory.	Visualization, analytics, machine learning that is compute or memory intensive but can be done on a single node.		Multi-node analytics jobs, jobs in reservations, custom project charging, and more.

Alternatively please use a reservation (details later)

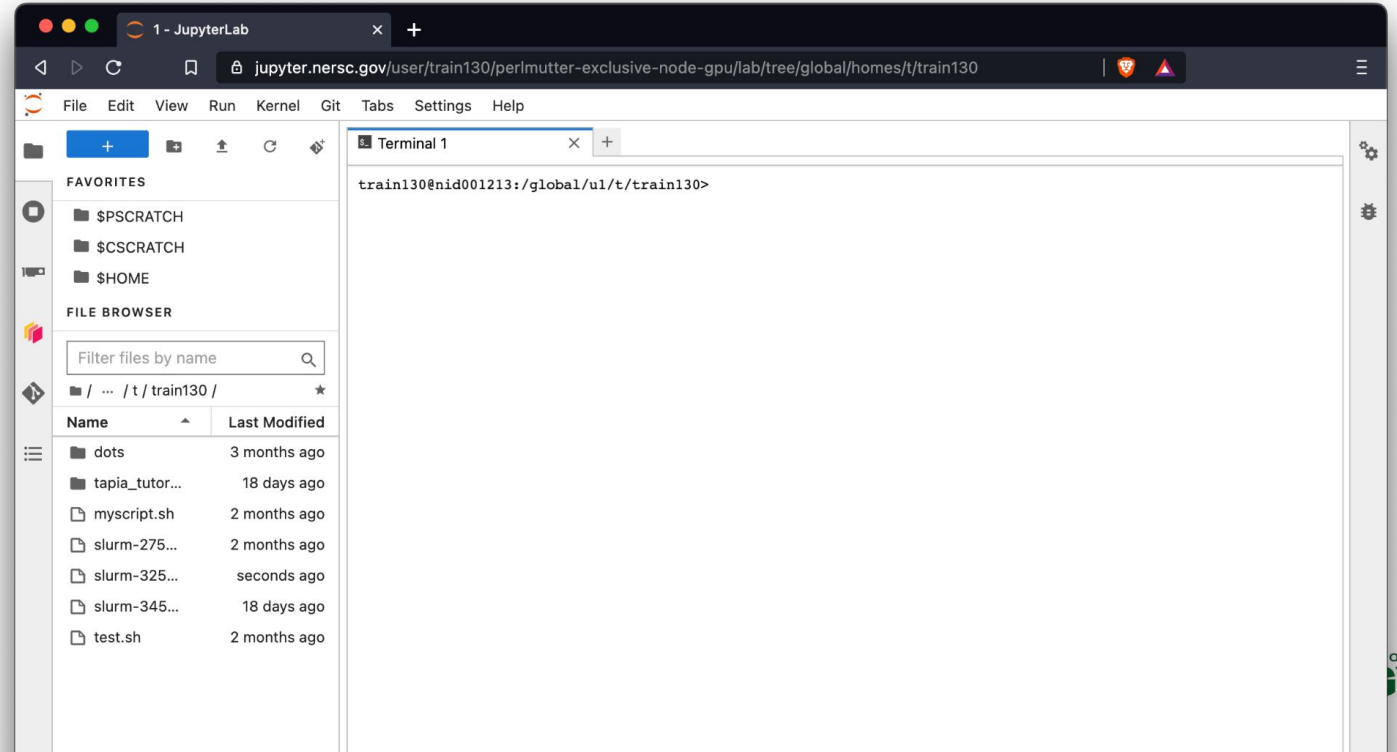
Setup

- Jupyter should take a minute to start:



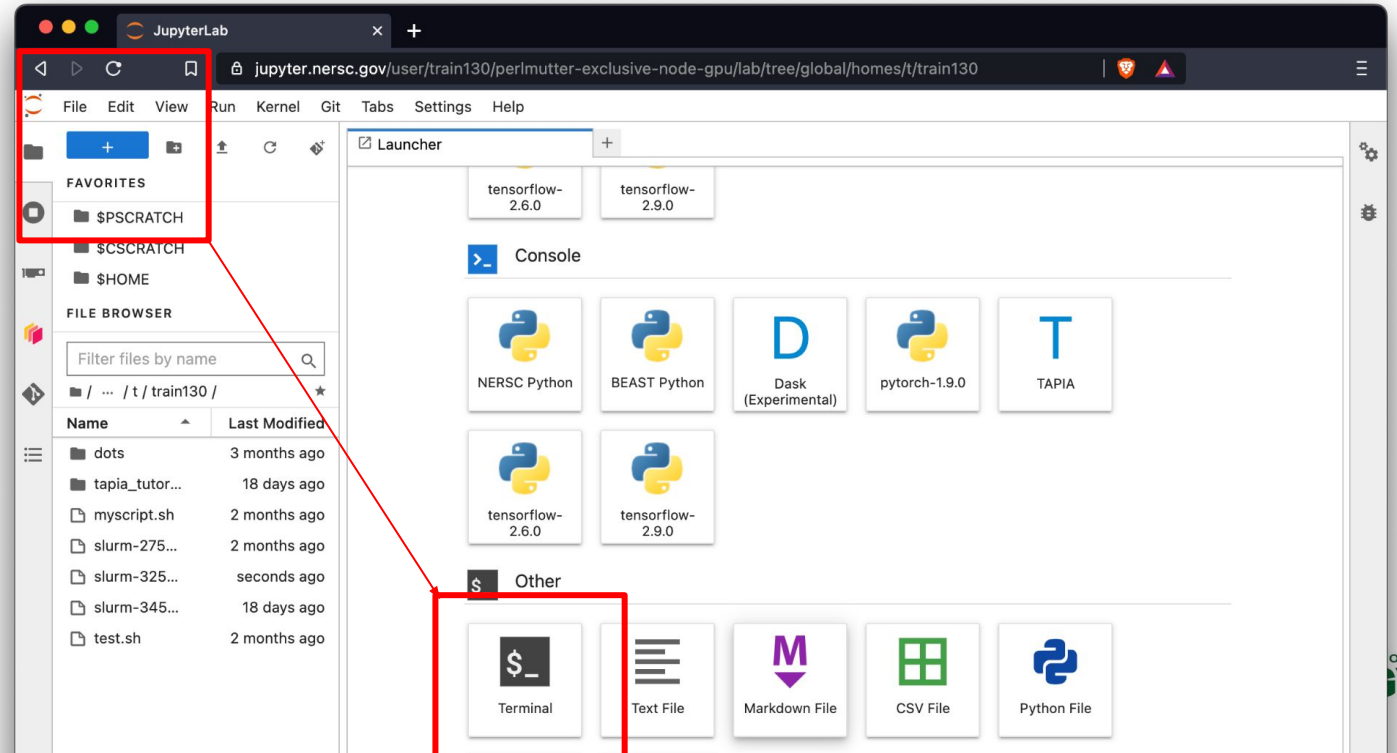
Setup

- Once started you should see a terminal



Setup

- (If you don't see a terminal), select "+" followed by "Terminal"

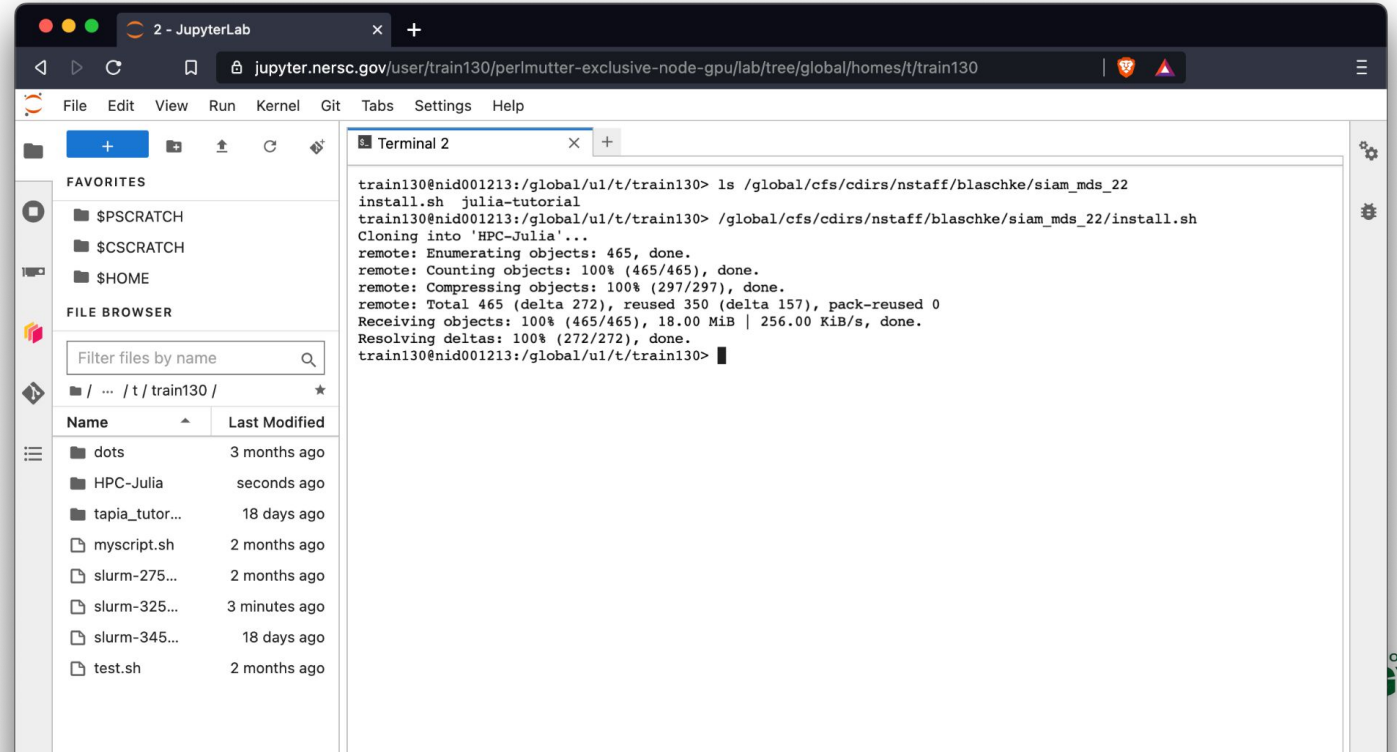


NERSC

Office of Science

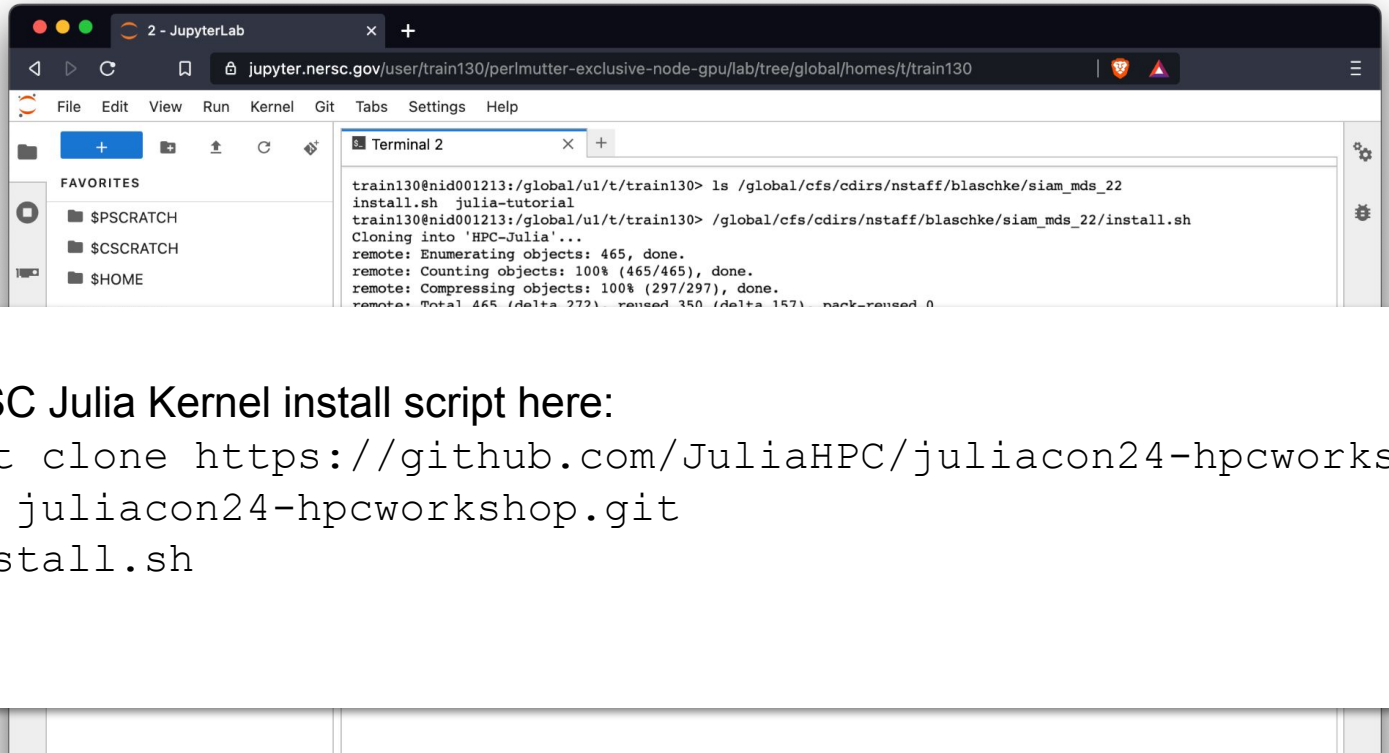
Setup

- (In the terminal), follow Carsten's installation instructions



Setup

- (In the terminal), follow William's installation instructions

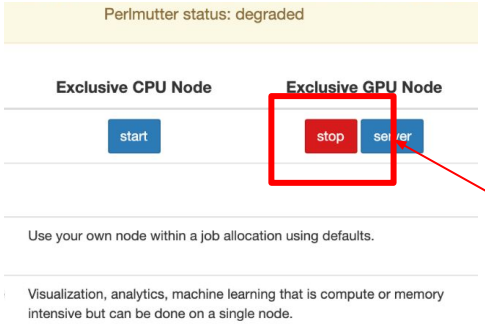


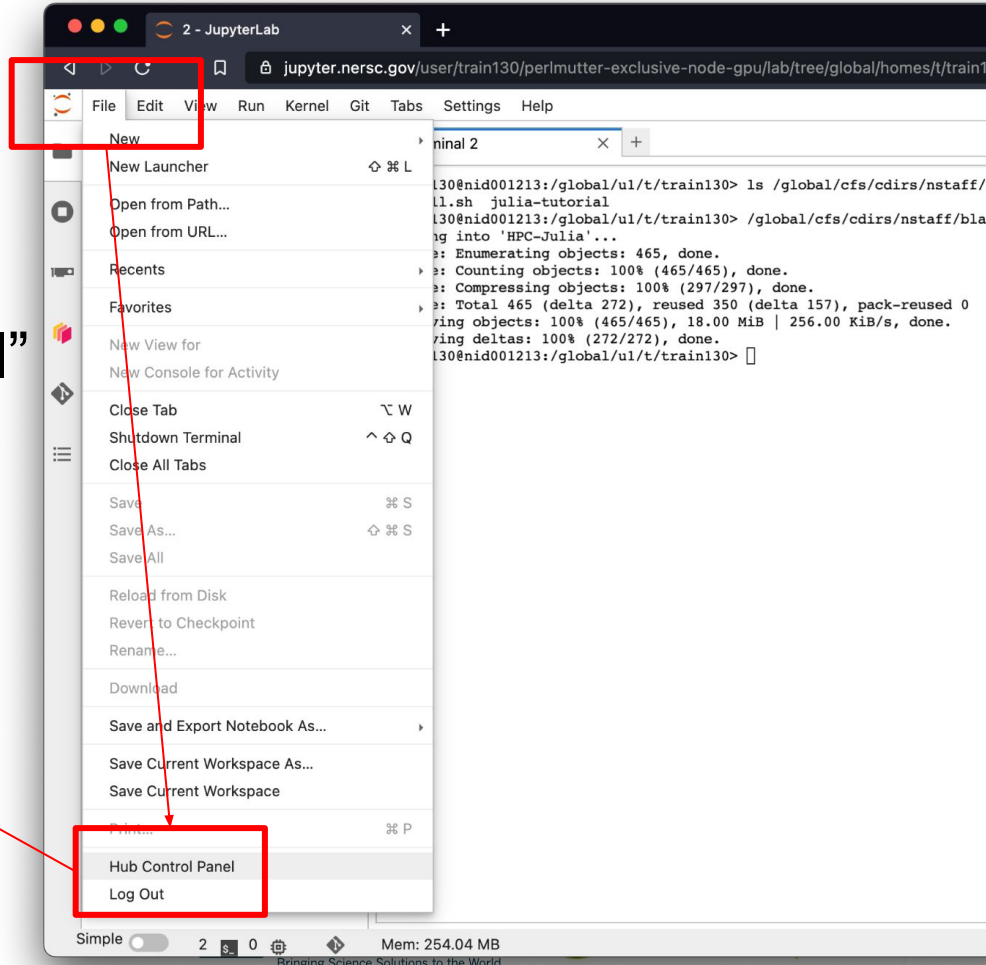
NERSC Julia Kernel install script here:

```
$ git clone https://github.com/JuliaHPC/juliacon24-hpcworkshop.git
$ cd juliacon24-hpcworkshop.git
$ install.sh
```

Setup

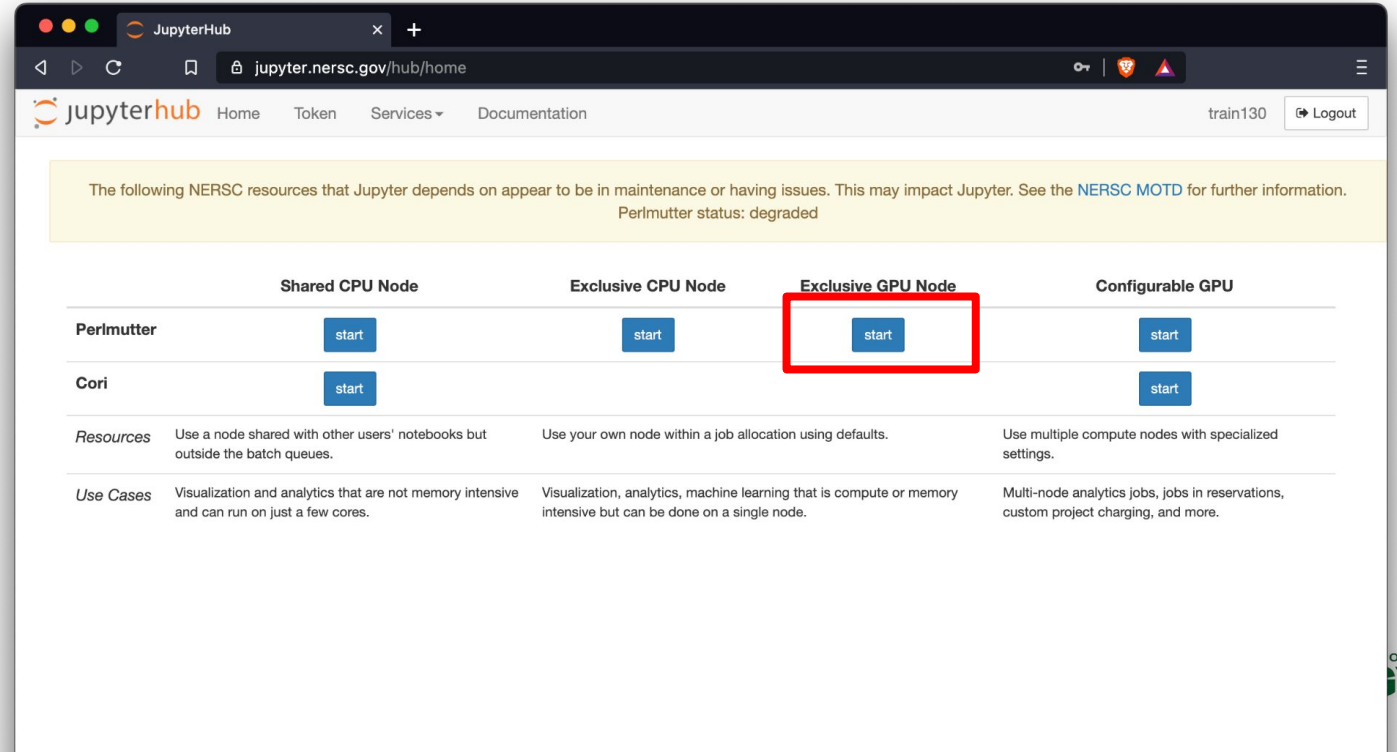
- Stop your server
  by going to:
  “File” > “Hub Control Panel”
- The selecting “Stop”





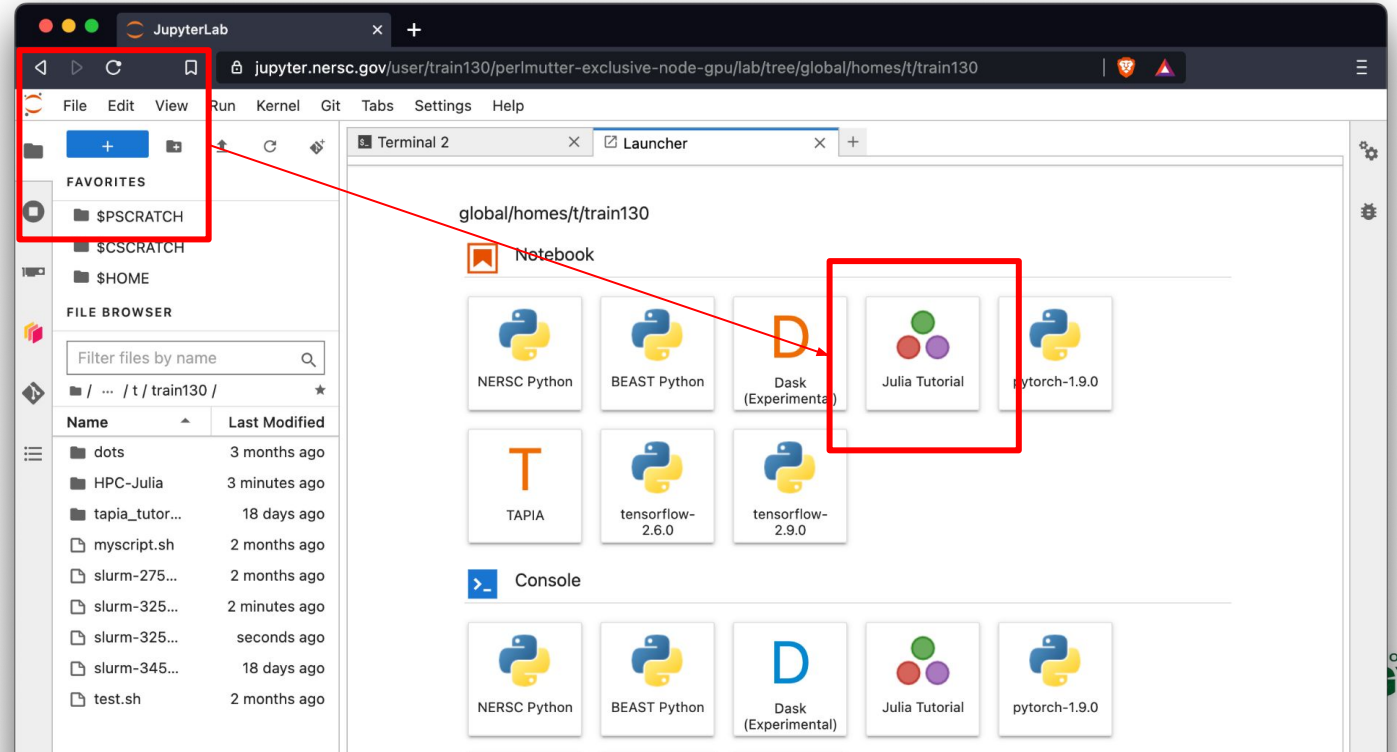
Setup

- Start a fresh exclusive node on Perlmutter



Setup

- Select the launcher, you should see the Julia Kernel :)

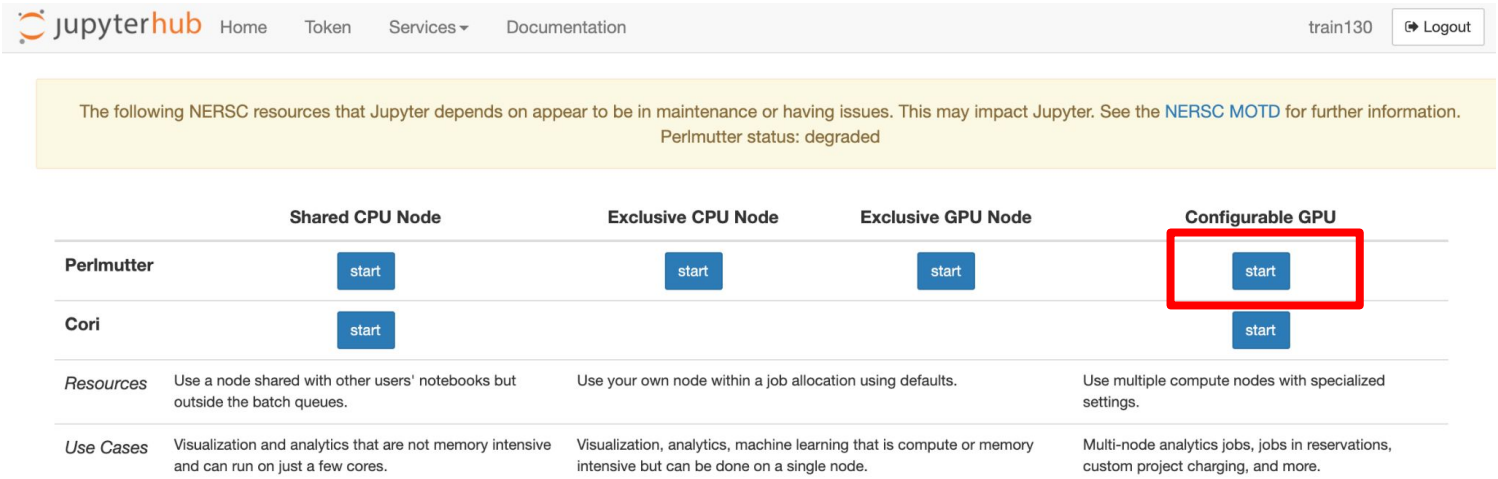


NERSC

Office of Science

Using Reservations in Tutorials

- Go to https://jupyter.nersc.gov and select: "Configurable GPU" in the "Perlmutter" row



Jupyter Options:

Leave defaults, except:

Account:

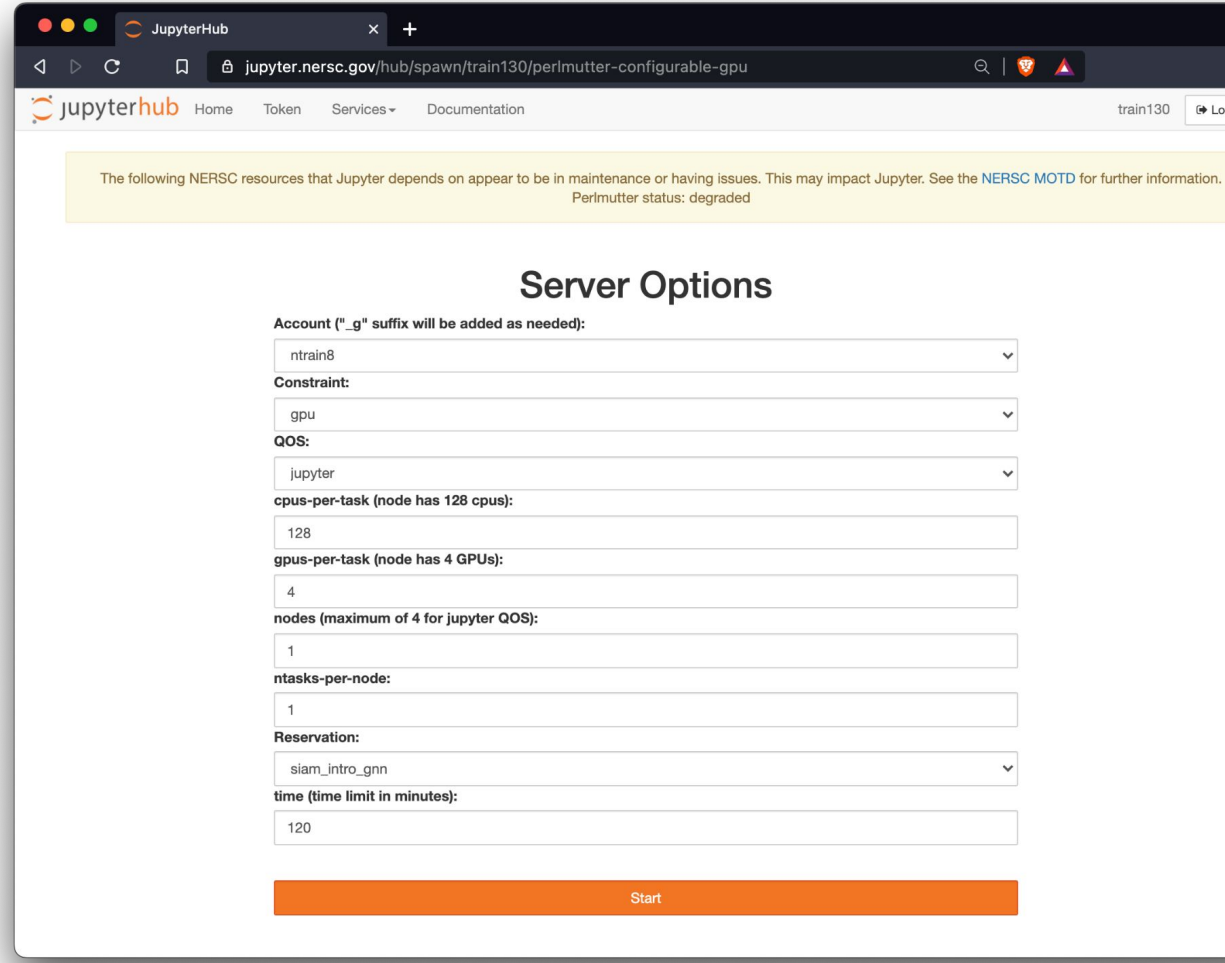
`ntrain1`

Reservation

`julia_traing`

Time

`180`



Note:

- Reservations now and run for 3 hours. If you request a node during this time, make sure that the current time + requested time does not exceed the reservation's end time.

- Training accounts are fully fledged NERSC accounts
- Will remain available until Sunday – please copy any data and code to your computer before then