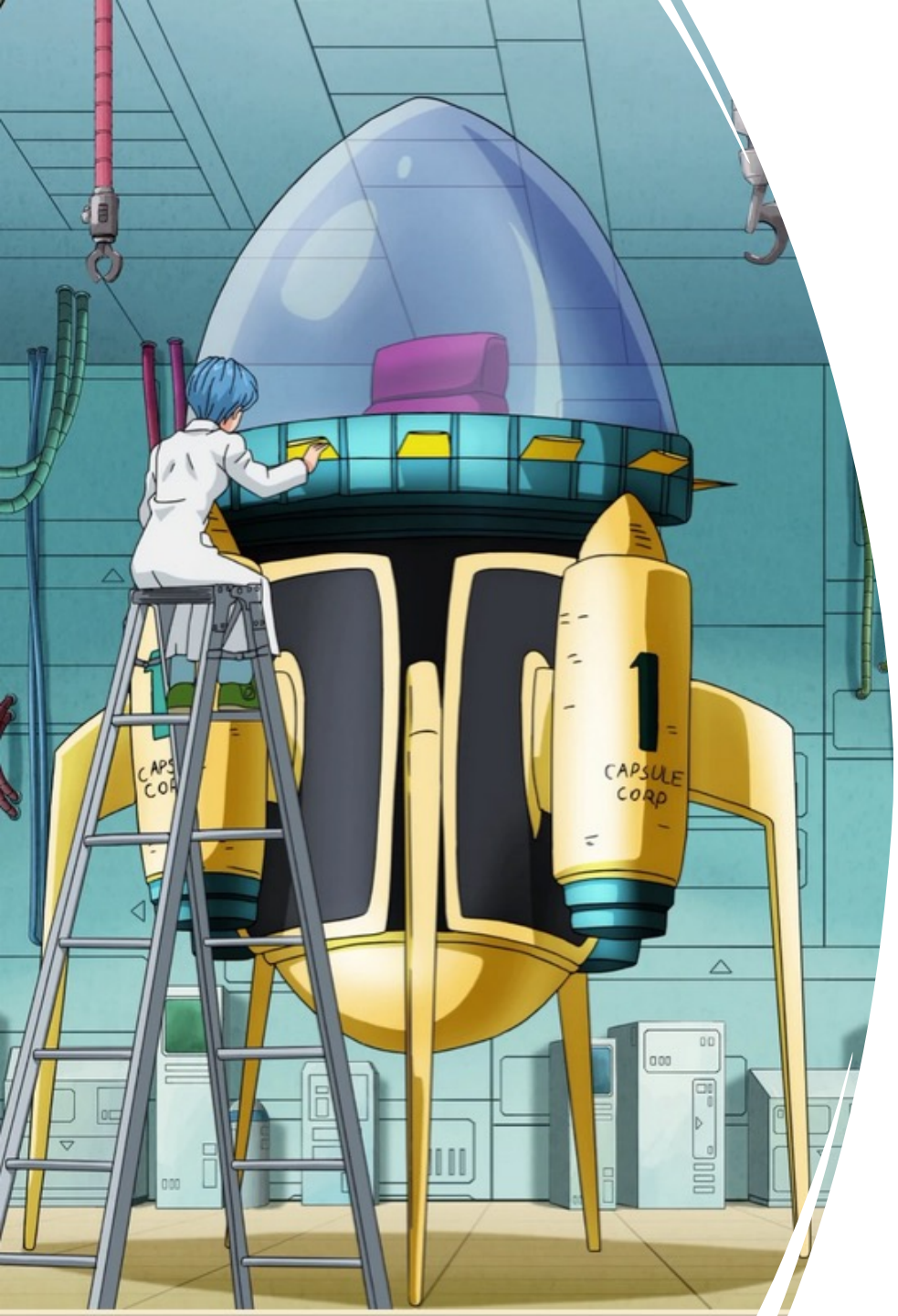
Introduction to Alpine

Kevin Fotso



I- Part 1) Elements of computing

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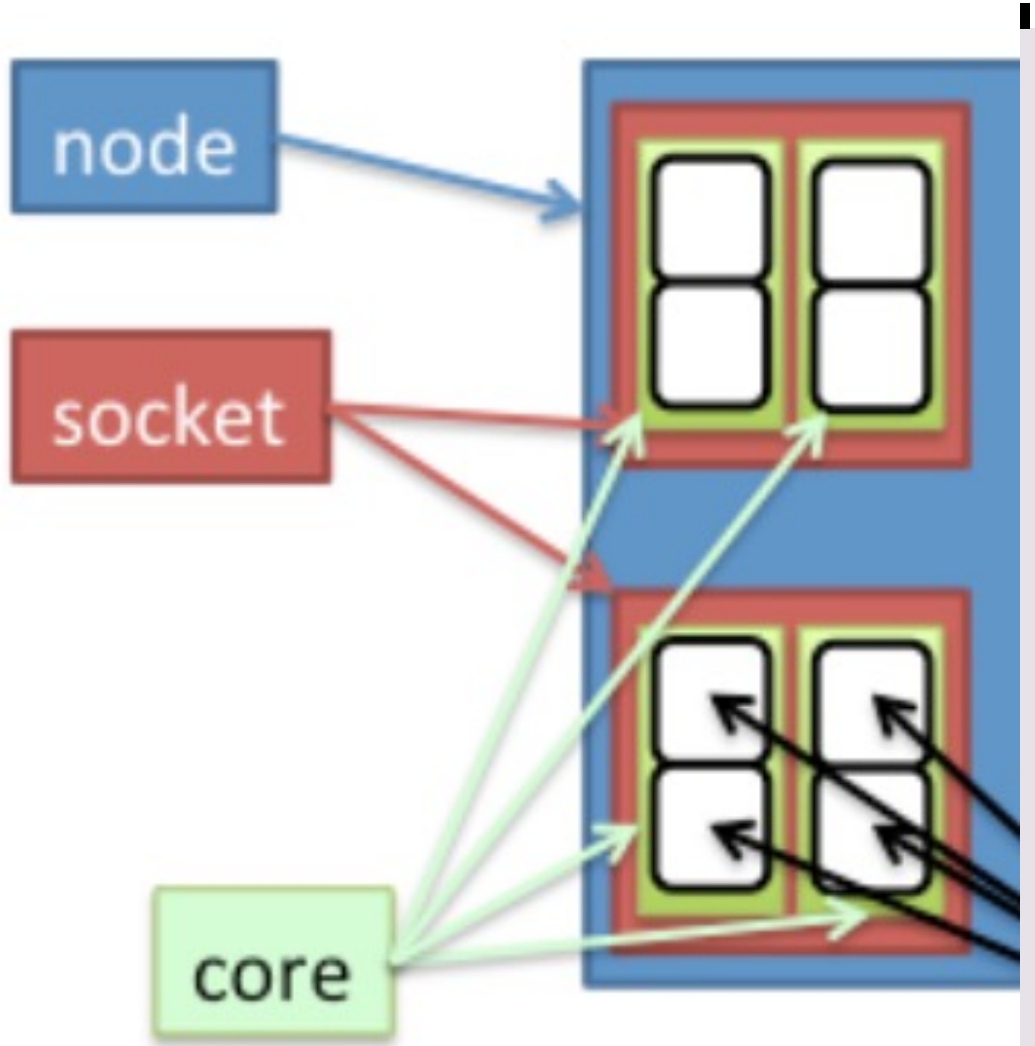
Parts of the processing chip (1)

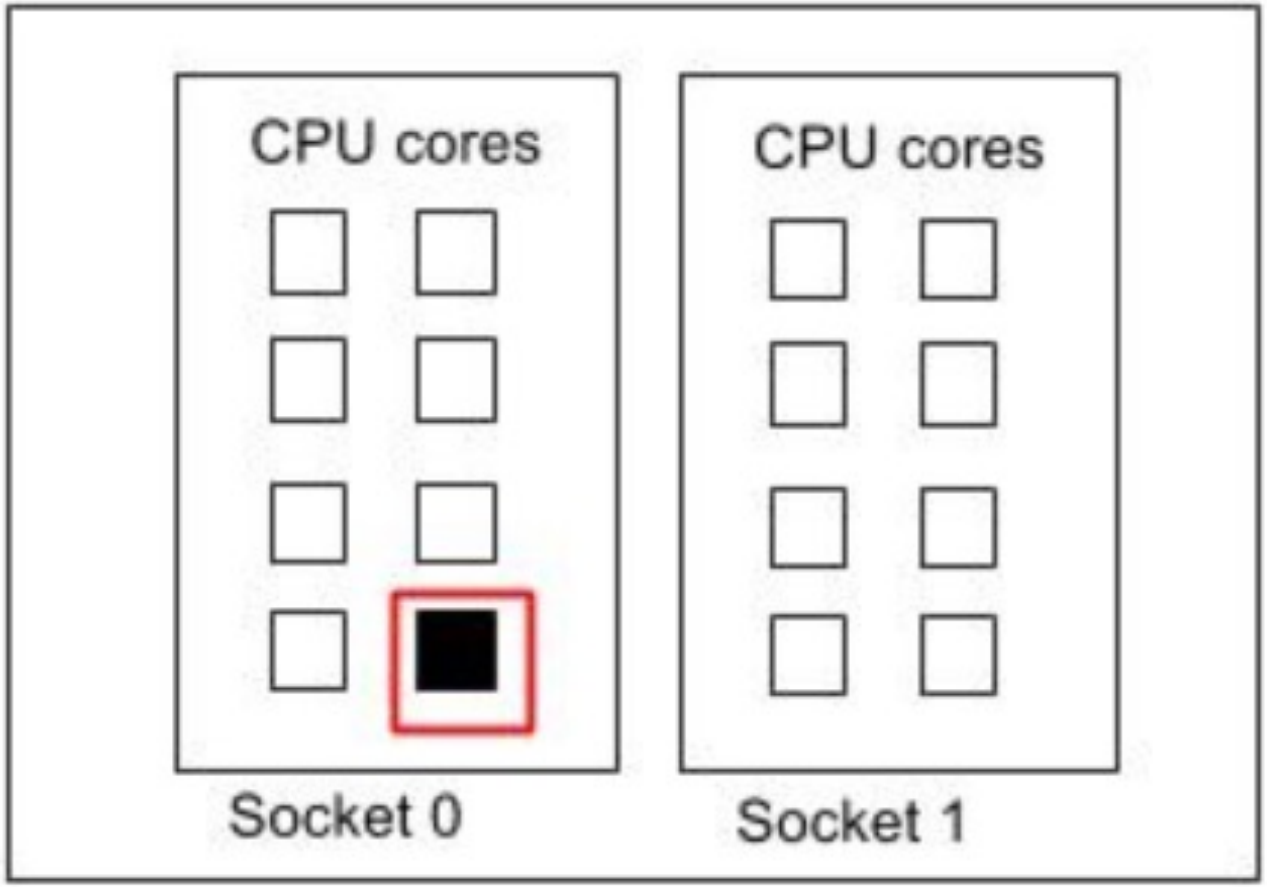
- A socket can be considered an entire computing chip in modern computers.
- Contains more than 1 core.
- On supercomputers a node usually contains more than 1 socket.

A core contains an Arithmetic and Logic Unit **(ALU)** + Registers

Parts of the processing chip (2)

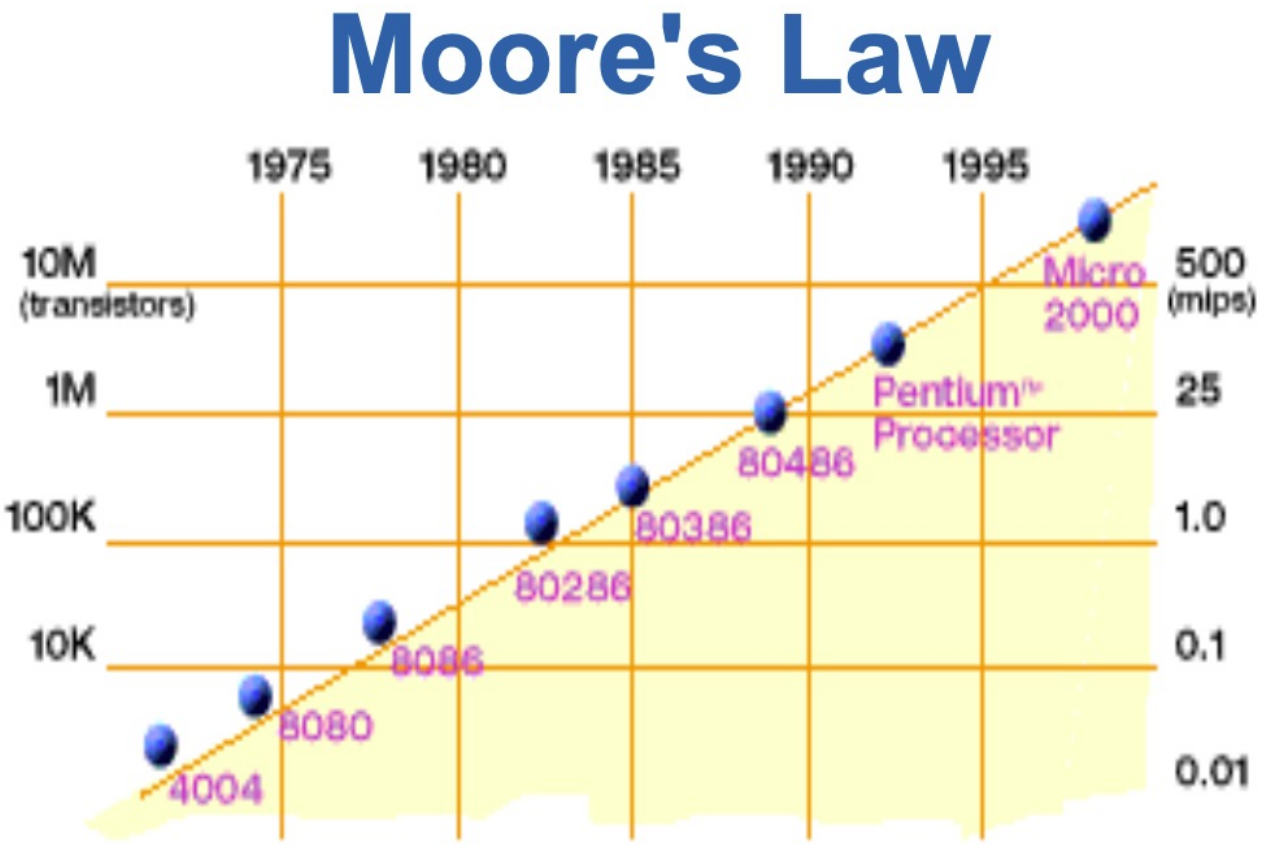


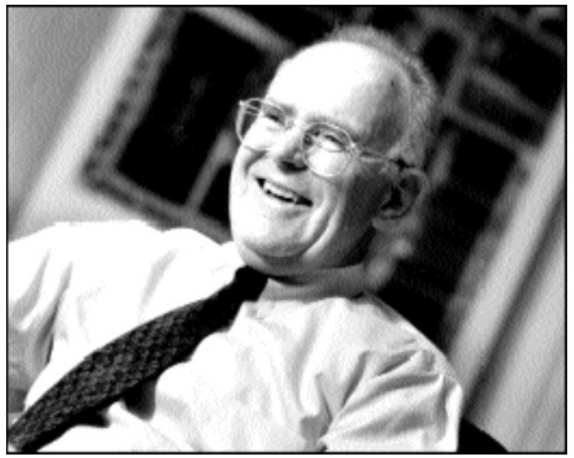
Parts of the processing chip (2)



Moore’s law (1)

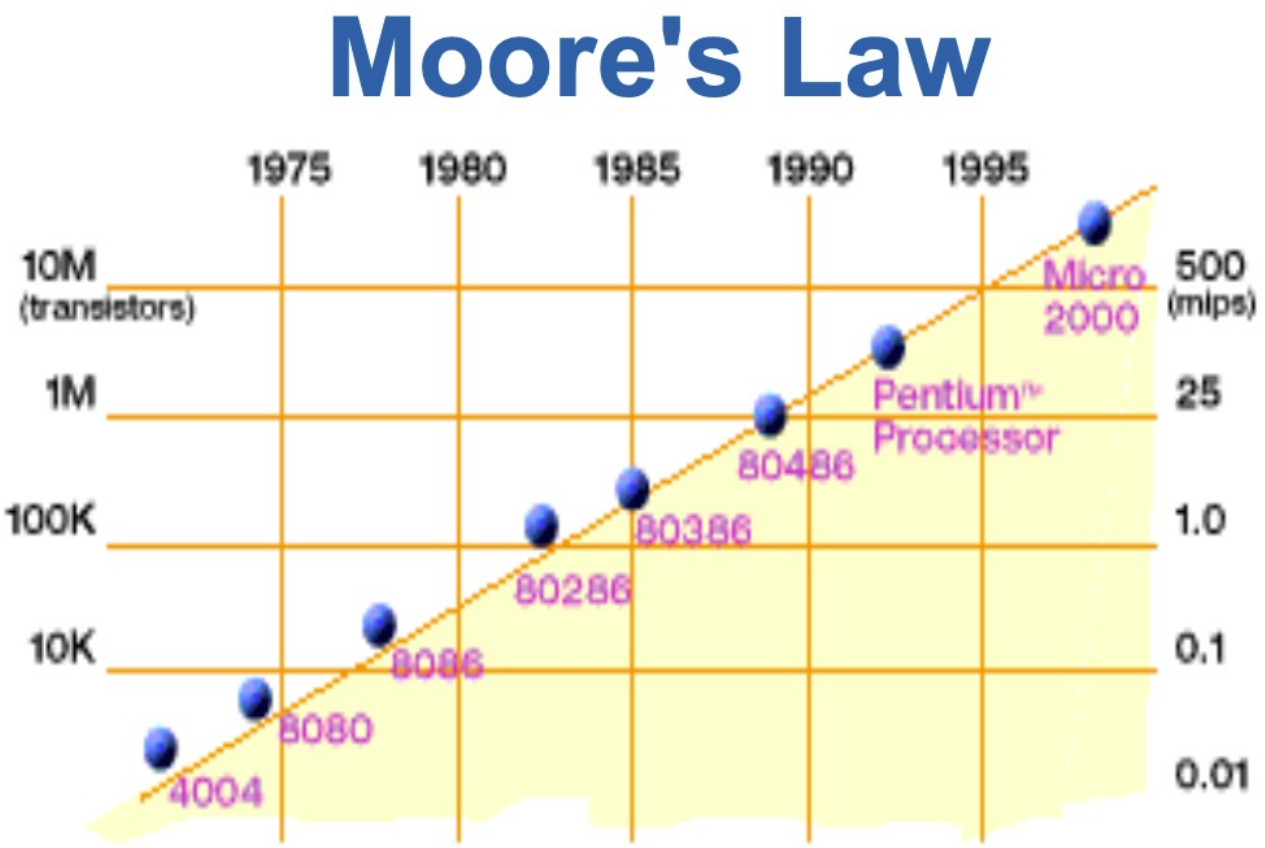
- Transistor count doubles in a chip every 18 months.

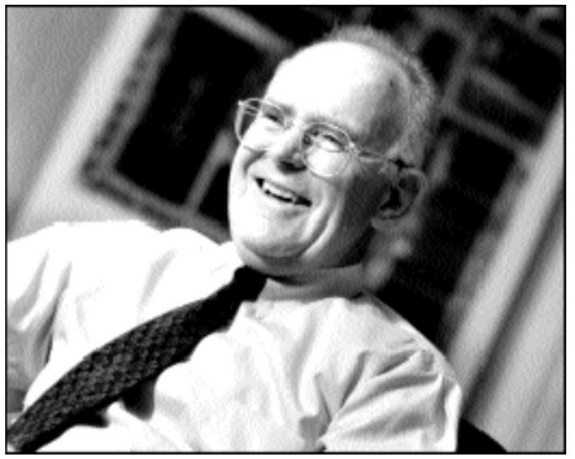




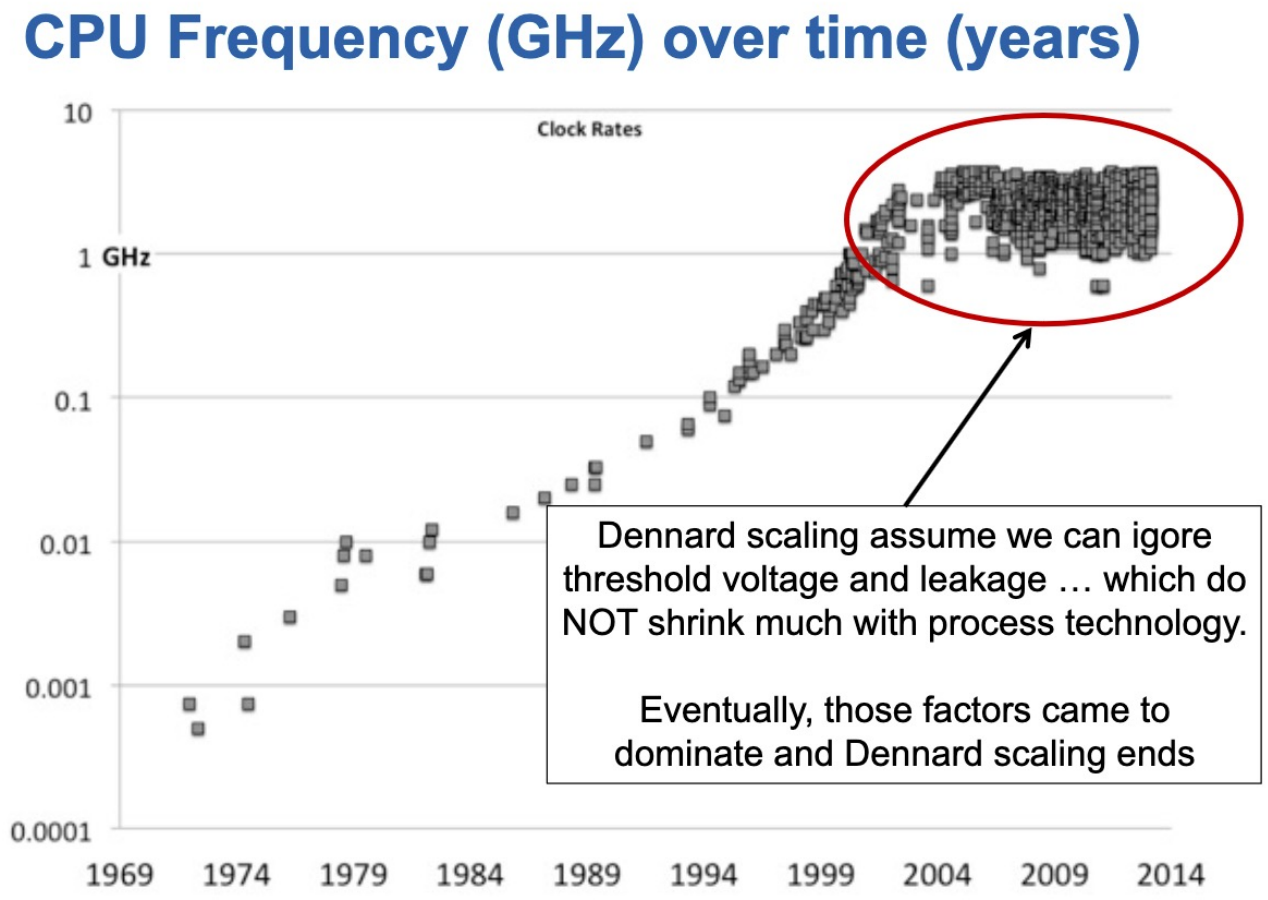
Moore’s law (2)

- Worked until around 2010 where it started to plateau



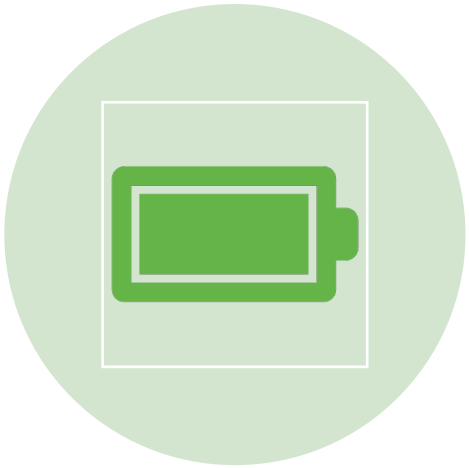


Moore's law plateau



- Number of cycles per seconds plateaued in the 2010s
- Why?

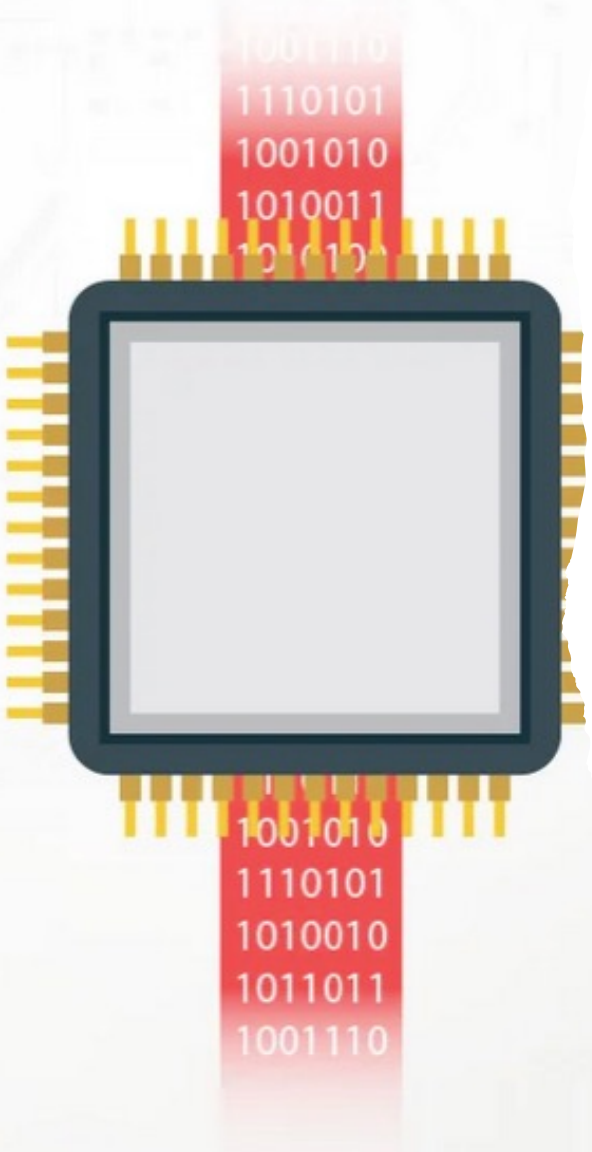
Why?



TRADITIONALLY, POWER DENSITY STAYS CONSTANT AS CHIPS FEATURE GOT SMALLER.

HOWEVER AROUND 2010, CLOCK FREQUENCY COULD NOT BE RAISED FURTHER BECAUSE THE HEAT DISSIPATION OR POWER WOULD HAVE GONE TOO FAR.

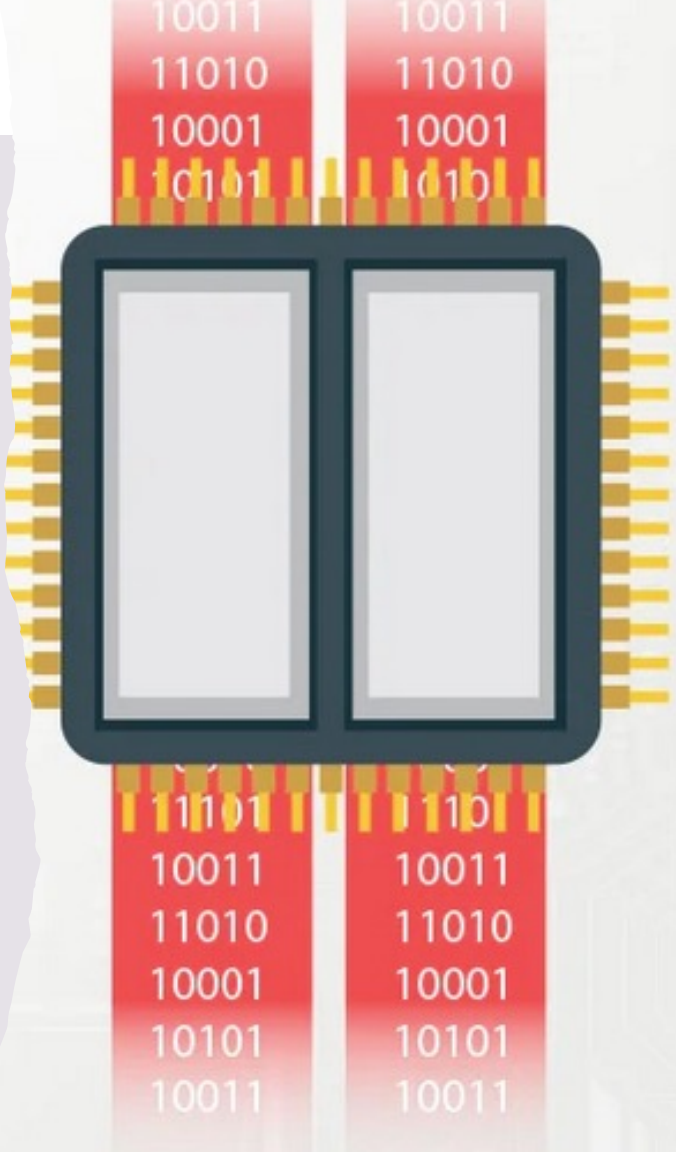
Increase need of parallelism



Single-core

Reduce power by adding cores of small frequency

2 cores at half frequency f can achieve the same throuput as a single core of frequency f



Dual Core

A look at an HPC cluster(1)

- Frontier supercomputer OAK Ridge National lab.
  [AMD Instinct MI250X GPU; 8,699,904 Cores

- Most powerful at the moment benchmarking with Linpack (e.g. Ax=b)

Source: https://www.ornl.gov/news/frontier-supercomputer-debuts-worlds-fastest-breaking-exascale-barrier

A look at an HPC cluster(2)

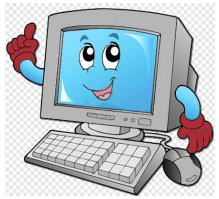
June 2023: The TOP 10 Systems (52% of the Total Performance of Top500)

Rank	Site	Computer	Country	Cores	Rmax [Pflops]	% of Peak	Power [MW]	GFlops/ Watt
1	DOE / OS Oak Ridge Nat Lab	Frontier, HPE Cray Ex235a, AMD 3rd EPYC 64C, 2 GHz, AMD Instinct MI250X, Slingshot 10	USA	8,699,904	1,194	71	22.7	52.6
2	RIKEN Center for Computational Science	Fugaku, ARM A64FX (48C, 2.2 GHz), Tofu D Interconnect	Japan	7,299,072	442.	82	29.9	14.8
3	EuroHPC /CSC	LUMI, HPE Cray EX235a, AMD 3rd EPYC 64C, 2 GHz, AMD Instinct MI250X, Slingshot 10	Finland	1,268,736	304.	72	2.94	52.3
4	EuroHPC/CINECA	BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 (108C), Quad-rail NVIDIA HDR100	Italy	1,824,768	239.	78	7.4	32.2
5	DOE / OS Oak Ridge Nat Lab	Summit, IBM Power 9 (22C, 3.0 GHz), NVIDIA GV100 (80C), Mellonox EDR	USA	2,397,824	149.	74	10.1	14.7
6	DOE / NNSA L Livermore Nat Lab	Sierra, IBM Power 9 (22C, 3.1 GHz), NVIDIA GV100 (80C), Mellonox EDR	USA	1,572,480	94.6	75	7.44	12.7
7	National Super Computer Center in Wuxi	Sunway TaihuLight, SW26010 (260C), Custom Interconnect	China	10,649,000	93.0	74	15.4	6.05
8	DOE / OS NERSC - LBNL	Perlmutter HPE Cray EX235n, AMD EPYC 64C 2.45GHz, NVIDIA A100, Slingshot 10	USA	706,304	64.6	71	2.59	27.4
9	NVIDIA Corporation	Selene NVIDIA DGX A100, AMD EPYC 7742 (64C, 2.25GHz), NVIDIA A100 (108C), Mellanox HDR	USA	555,520	63.4	80	2.64	23.9
10	National Super Computer Center in Guangzhou	Tianhe-2A NUDT, Xeon (12C) , MATRIX-2000 (128C) + Custom Interconnect	China	4,981,760	61.4	61	18.5	3.32

- Alpine has >18,000 cores!

Source: https://extremecomputingtraining.anl.gov/wp-content/uploads/sites/96/2023/08/ATPESC-2023-Track-4-AfterDinnerTalk-Dongarra-GrowingupatANL.pdf

Anatomy of supercomputing



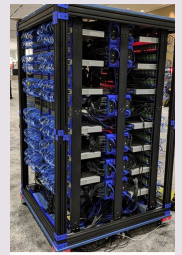
Laptop or PC

Login node

Slurm: scheduler

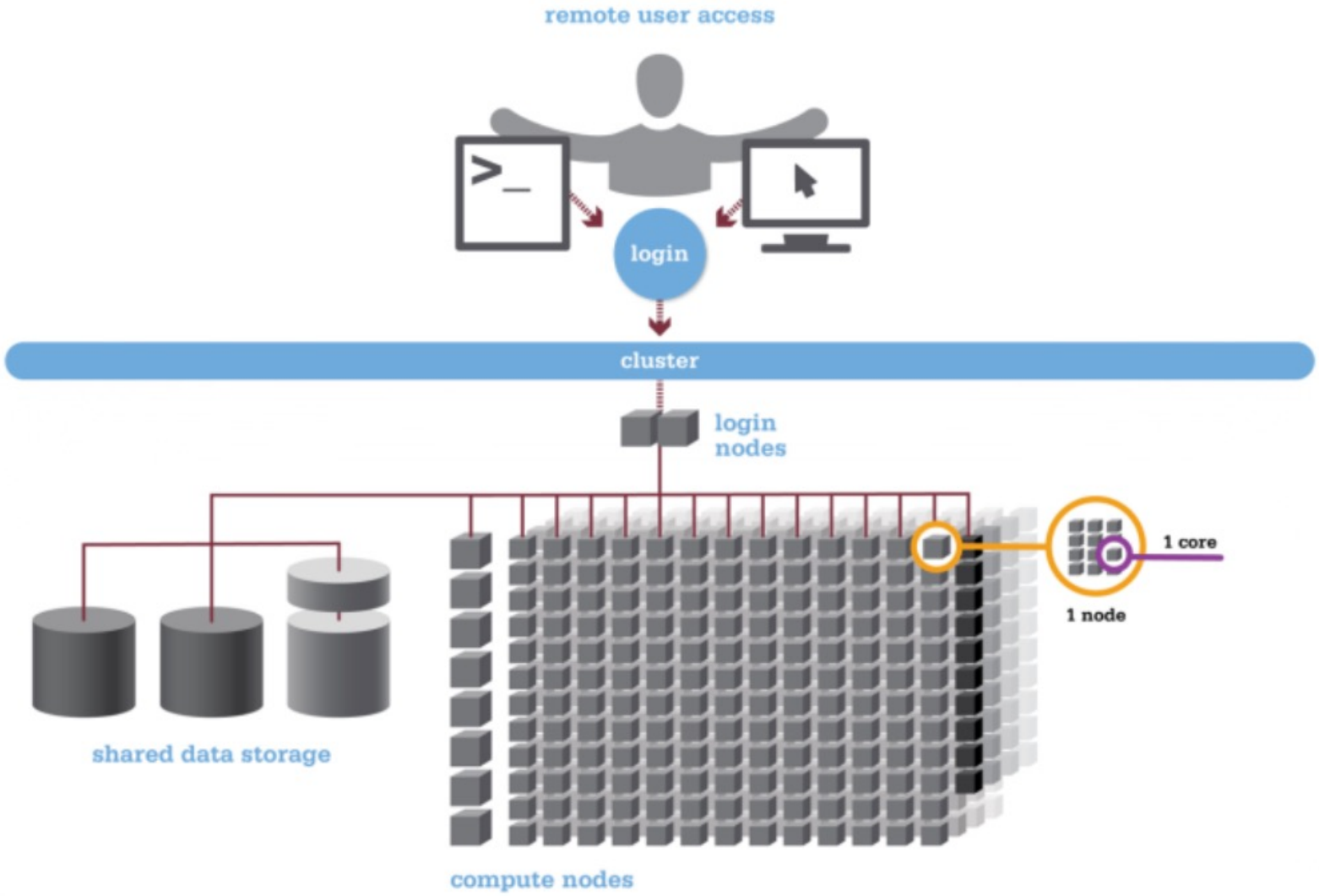
Fast interconnect

Storage



Compute node

Architechture of a supercomputer



- Login nodes. To log into the system, cd into directories, look at files etc ...
- Compute node. Dedicated to do the computation
- The slurm scheduler controls access to the compute nodes to avoid a tragedy of the commons ...

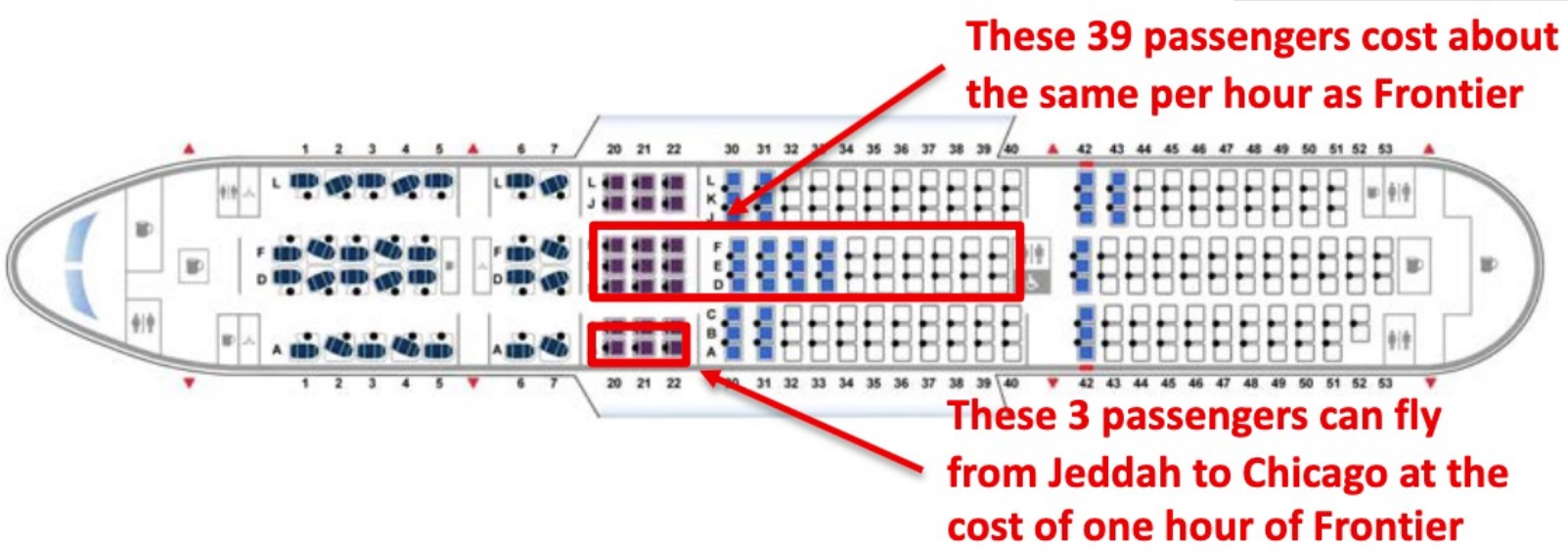
Why Slurm?

– Allows for better tracking of resource used per user

– Better management of of resource across user base

– More sustainable and less tragedy of the commons

– Widely used and supported by applications in case of bugs.



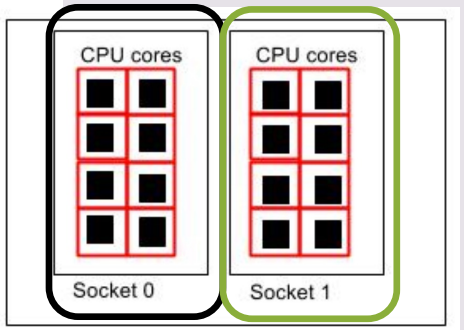
Source: https://extremecomputingtraining.anl.gov/wp-content/uploads/sites/96/2023/08/ATPESC-2023-Track-2b-Dinnerspeaker-Keyes-Efficient-Computation.pdf

Why Slurm?

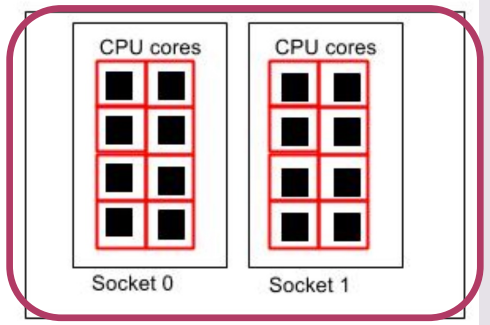
- Bulma request 8 cores from Node 1
- Dr. Brief requests 8 cores as well from Node 1
- Gohan requests 16 cores from Node 2
- No tragedy of the common!!!

Slurm scheduler

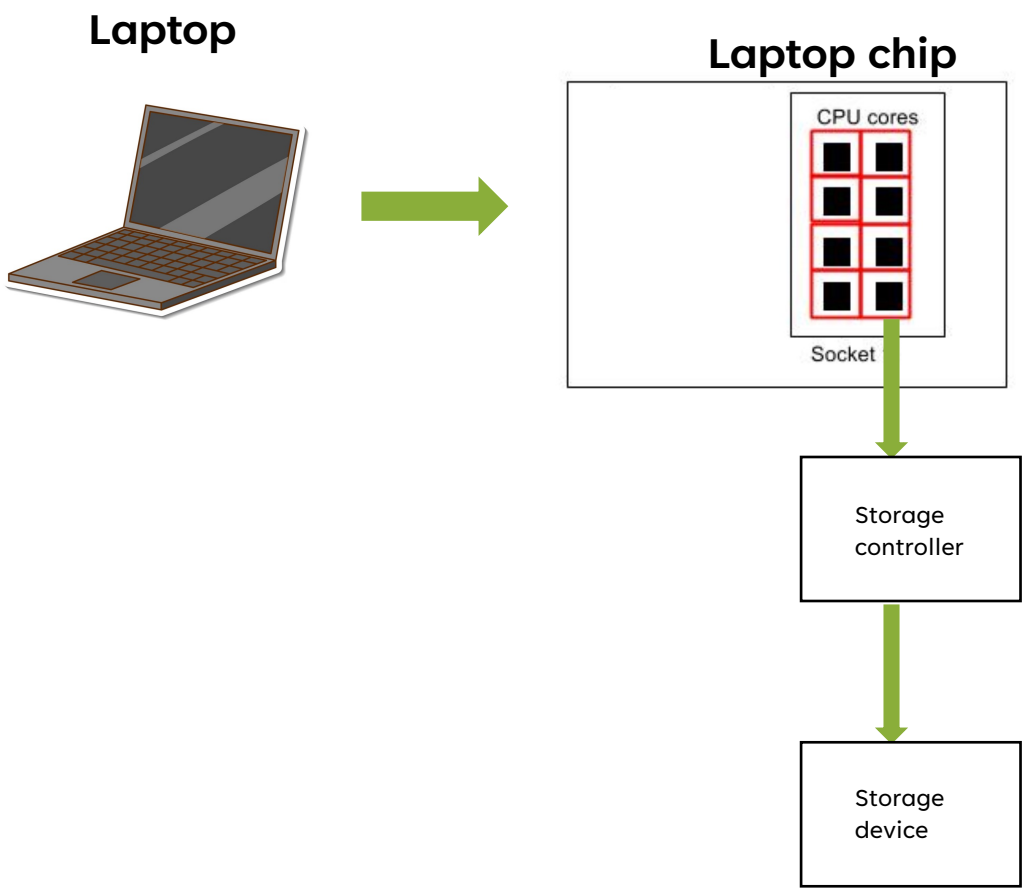
Node 1



Node 2



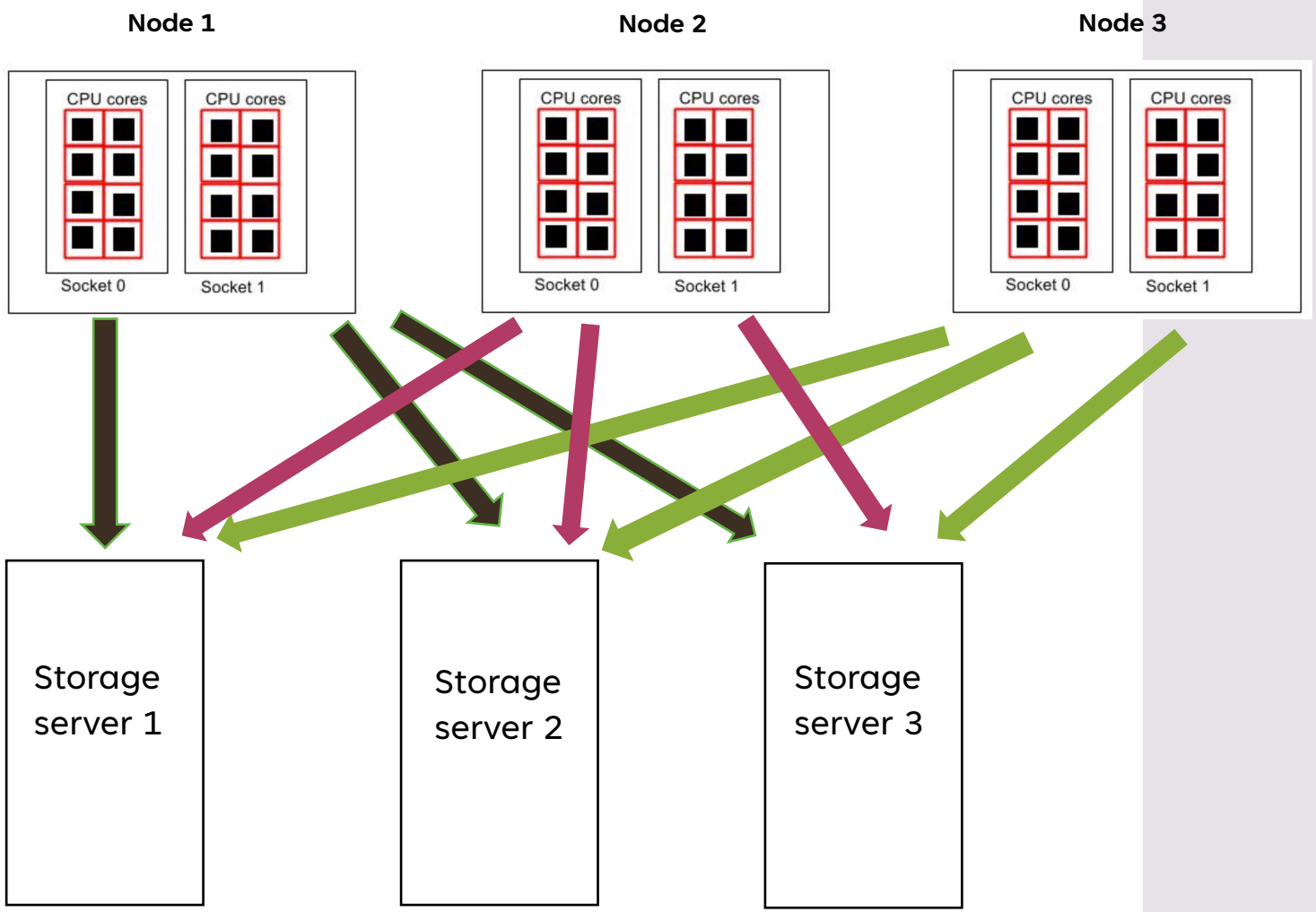
Overview of storage [PC]



- Compute core talks to the storage controller which talks to the storage device to get the data
- Path between software to storage is short.
- Low latency and low bandwidth.

Source: https://extremecomputingtraining.anl.gov/wp-content/uploads/sites/96/2023/08/ATPESC-2023-Track-7-Talk-2-carns-io-principles.pdf

Overview of storage [HPC]



- Files distributed across multiple servers.
- Much Higher bandwidth.
- In general higher latency.

Source: https://extremecomputingtraining.anl.gov/wp-content/uploads/sites/96/2023/08/ATPESC-2023-Track-7-Talk-2-carns-io-principles.pdf

Filesystems on High Performance Computing

- Network filesystem (NFS): Allows users to access files and directories located on remote servers

GPFS High performance filesystem

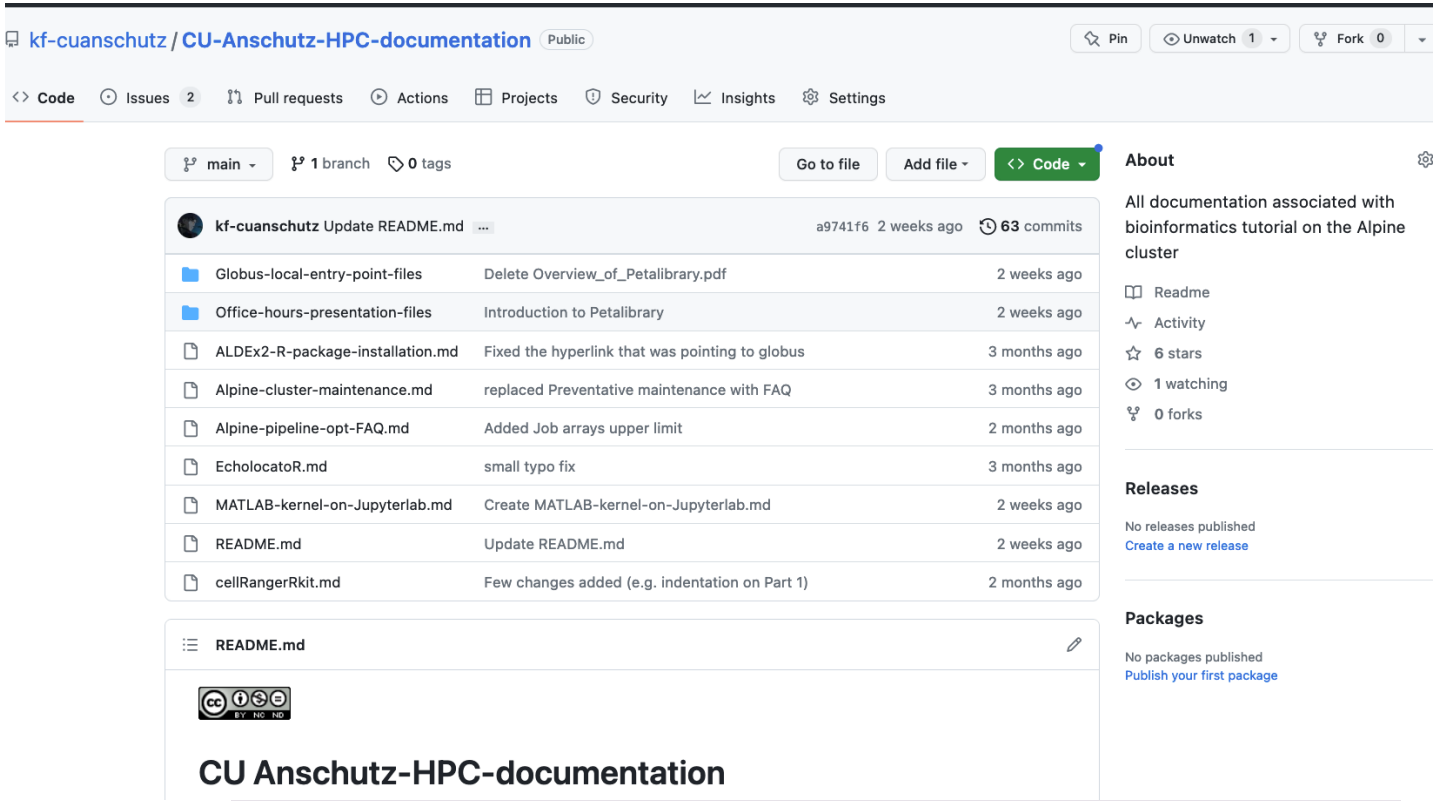
- Optimized for heavy I/O pipelines
- Optimized for heavy parallelized pipelines

II- Part 2) Intro to Alpine

Official Github pages:

– CU Anschutz HPC official Github page:

https://github.com/kf-cuanschutz/CU-An documentation.



- Note: You can submit pull requests as well.

– CU Boulder curc doc:

https://curc.readthedocs.io/en/latest/access/logging-in.html

- Tickets submitted by emailing: rc-help@olorado.edu. You may email AMC HPC Support as well: hpcsupport@cuanschutz.edu.

Logging into Alpine(1)

Alpine Office Hours_.pdf
422 KB

<User Name>,
Congratulations on your new Alpine account! You are now ready to start using Alpine.

To help you navigate Alpine and get your workflows started quickly. we have compiled a few quick instructions and tips on how to get the most out of your experience. For a fully comprehensive overview of all documentation related to Alpine, please visit the following site: https://curc.readthedocs.io/en/latest/index.html. We recommend you bookmark this site and save this email message for future use.

Please note, all functionality, commands, and directives can only be used after requesting an acompile node on the command line. This can be done by typing `acompile` and pressing enter once you are logged into the terminal. From there, all SLURM and module commands will work as expected.

Introduction to the SLURM job scheduler
Alpine utilizes the SLURM job scheduling software to manage job submissions to the compute nodes. The Boulder CURC team has provided tutorials and documentation for how to write your job scripts in order for the head node to allocate and assign your jobs with the appropriate resources you are requesting.

- Useful SLURM script examples: https://curc.readthedocs.io/en/latest/clusters/alpine/examples.html
- Commonly used SLURM commands on Alpine: https://curc.readthedocs.io/en/latest/running-jobs/slurm-commands.html
- SLURM flags and partitions on Alpine: https://curc.readthedocs.io/en/latest/running-jobs/job-resources.html
- How to write and submit a SLURM job script: https://curc.readthedocs.io/en/latest/running-jobs/batch-jobs.html
- Setting up an interactive job with SLURM: please use the `acompile` or `sinteractive` commands to spin up an interactive job; specify the -h flag to see all options for these commands.

All Anschutz users should specify `#SBATCH --account=amc-general` in their job submission scripts in order to get the Anschutz priority boost enabled on their jobs.

Logging into Alpine

- For Anschutz users, you will need to login to Alpine by following the set of instructions outlined here in this link using the Open OnDemand portal.
- For now, directly accessing Alpine from the terminal using ssh is not yet enabled. We will notify you when this feature is available.

Your directories on Alpine
The paths below use the built-in shell variable $USER to represent your username. You can access them directly using the paths shown below, since $USER will be replaced with your username by the shell. If you are unsure of your username, you can find it by typing `echo $USER` on the Alpine terminal. For Anschutz users, this may have the @xsede.org or @access.org extension.

/home/$USER

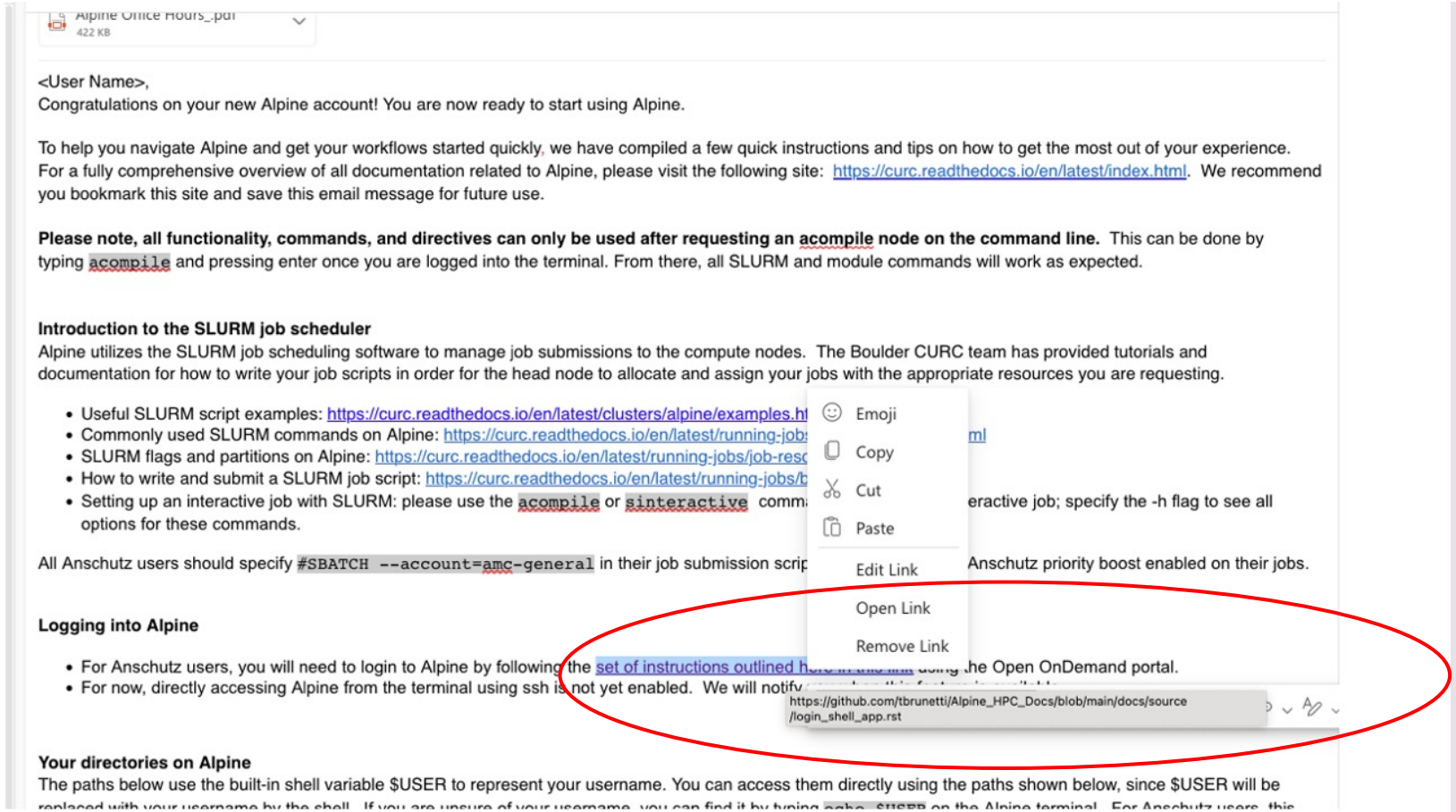
- 2 GB per user
- Not meant to be used for data storage or for reading and writing to/from compute nodes!
- It should be used for .bashrc, .bash_profile, .ssh, etc...

/projects/$USER

- 250 GB per user
- Used for very small data (<1 GB) and local software installs
- When compiling software, please use a compile node, not the head node. For more information on nodes please visit node types here.

- Once the user's EUA application is approved, they will receive an onboarding email similar to what is above.

Logging into Alpine(2)



- Then they will open the following link in listed in the email and follow the procedure.

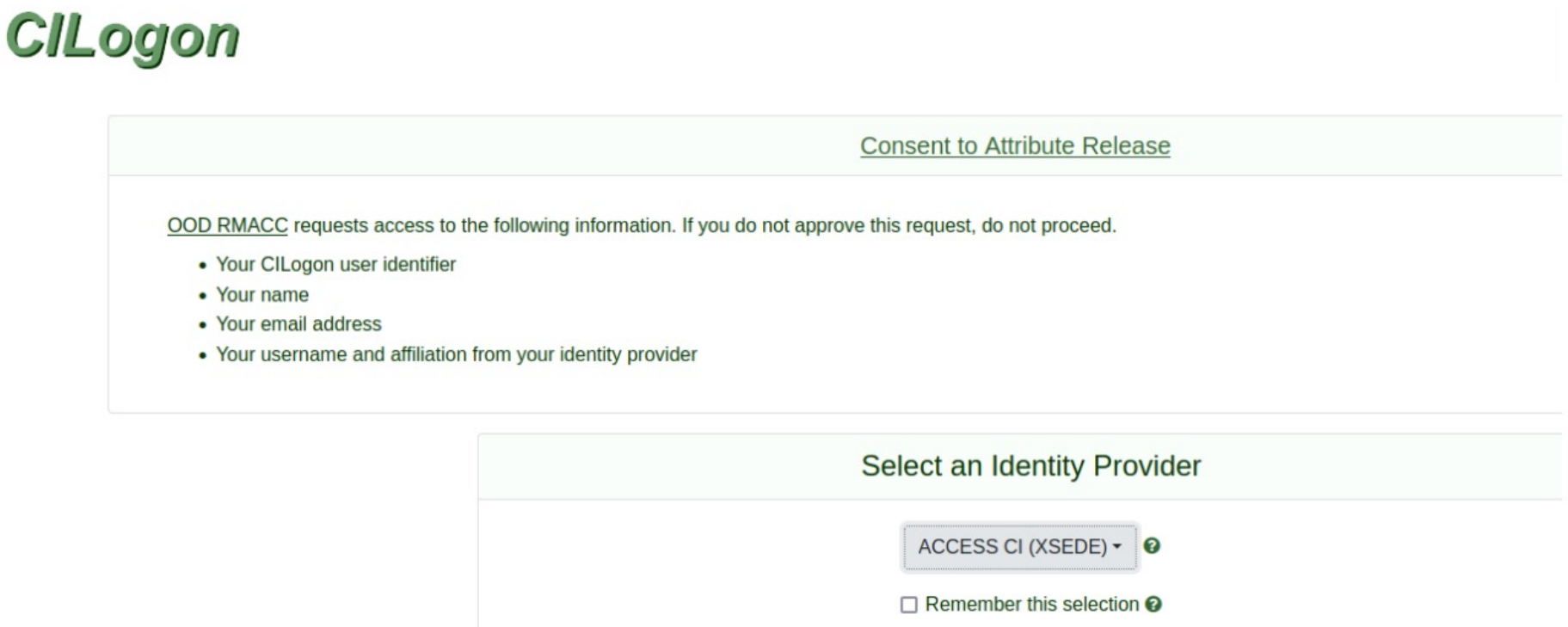
Logging into Alpine(3)

Logging into Alpine from the Shell App

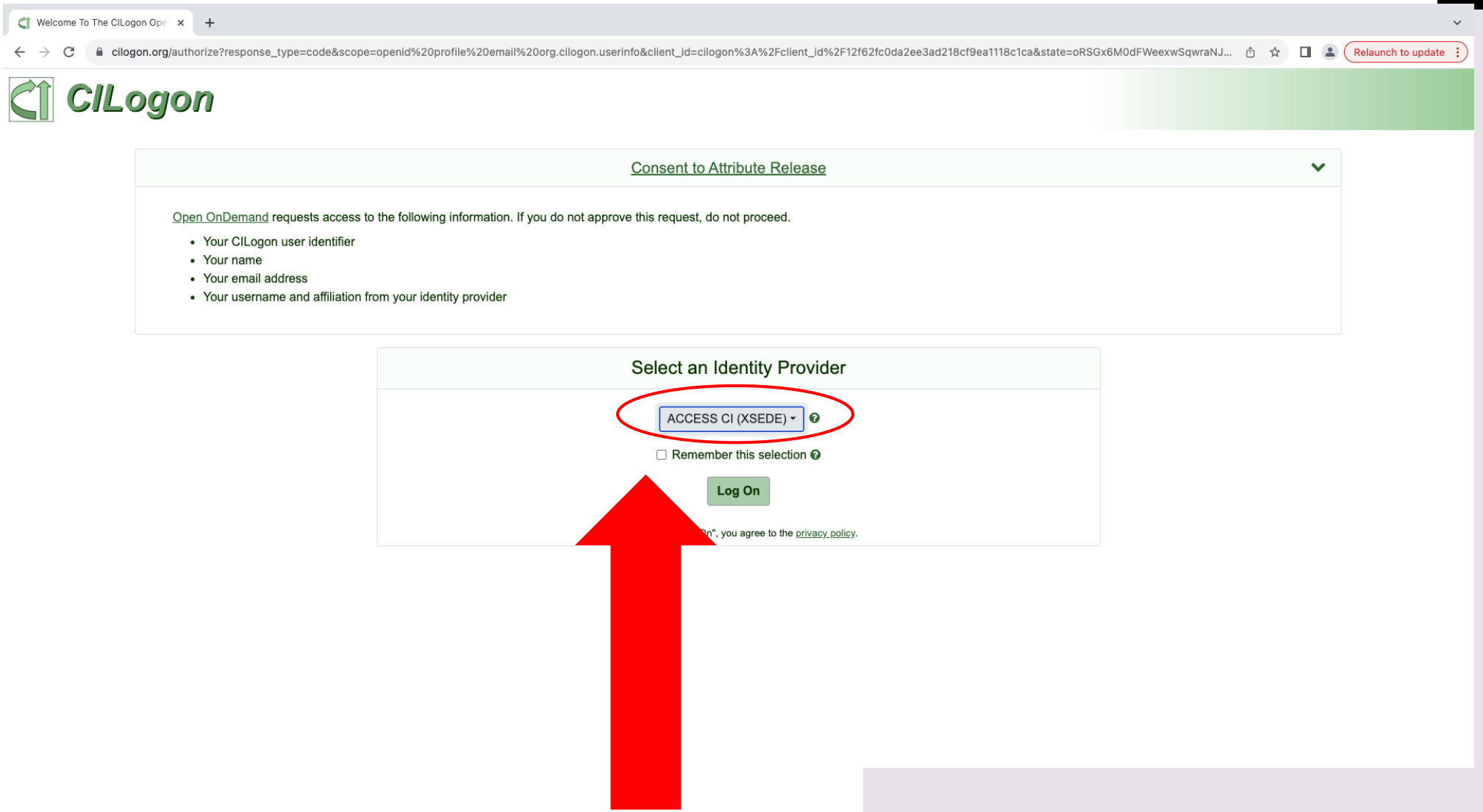
Note

Make sure you already have your XSEDE/ACCESS user name and password set up before proceeding and Duo 2-factor authentication set up for your ACCESS/XSEDE account

1. Visit https://ondemand-rmacc.rc.colorado.edu . You will be redirected to CILogon. From there, make sure you select the ACCESS CI (XSEDE) as your identity provider and then click the "Log On" button.

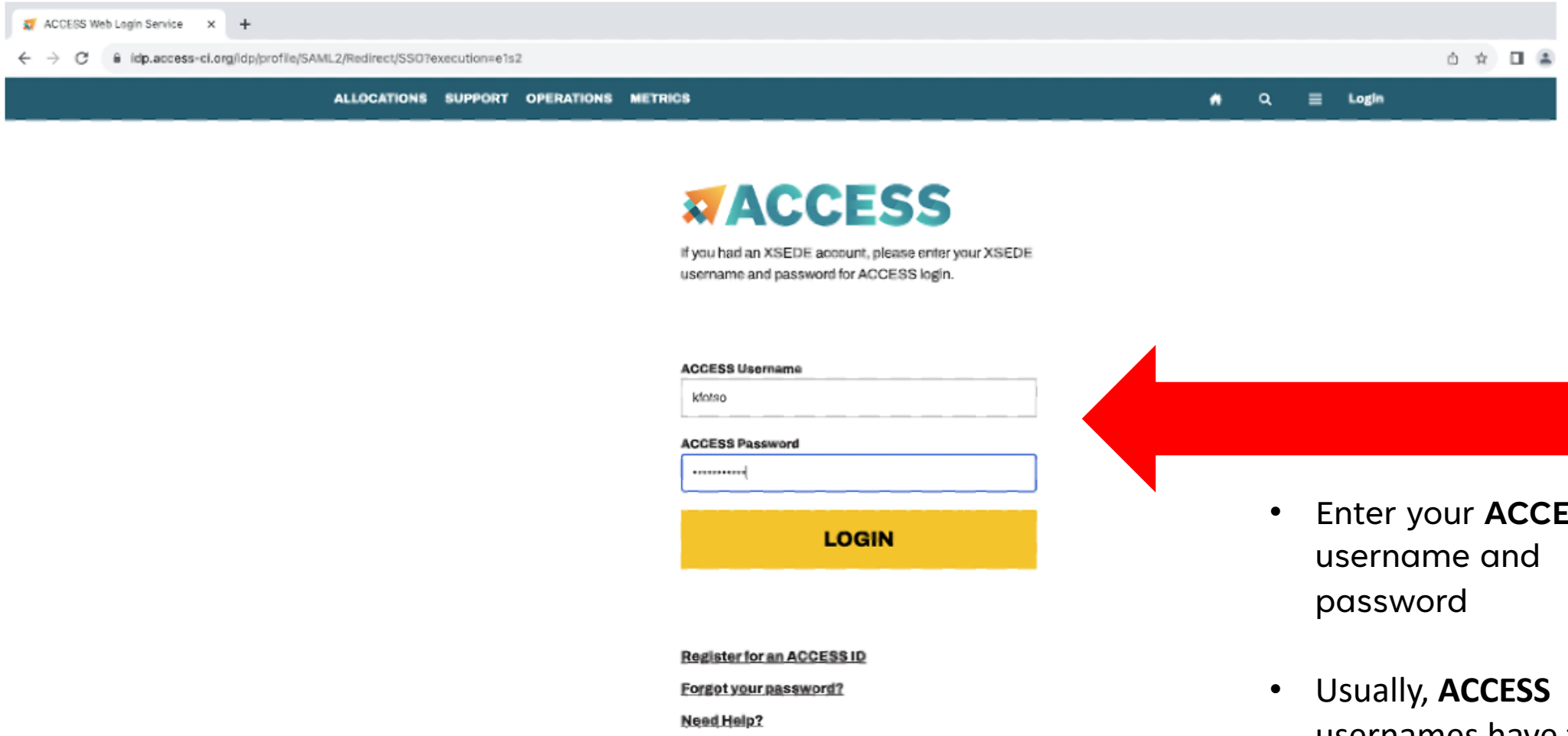


Logging into Alpine(4)



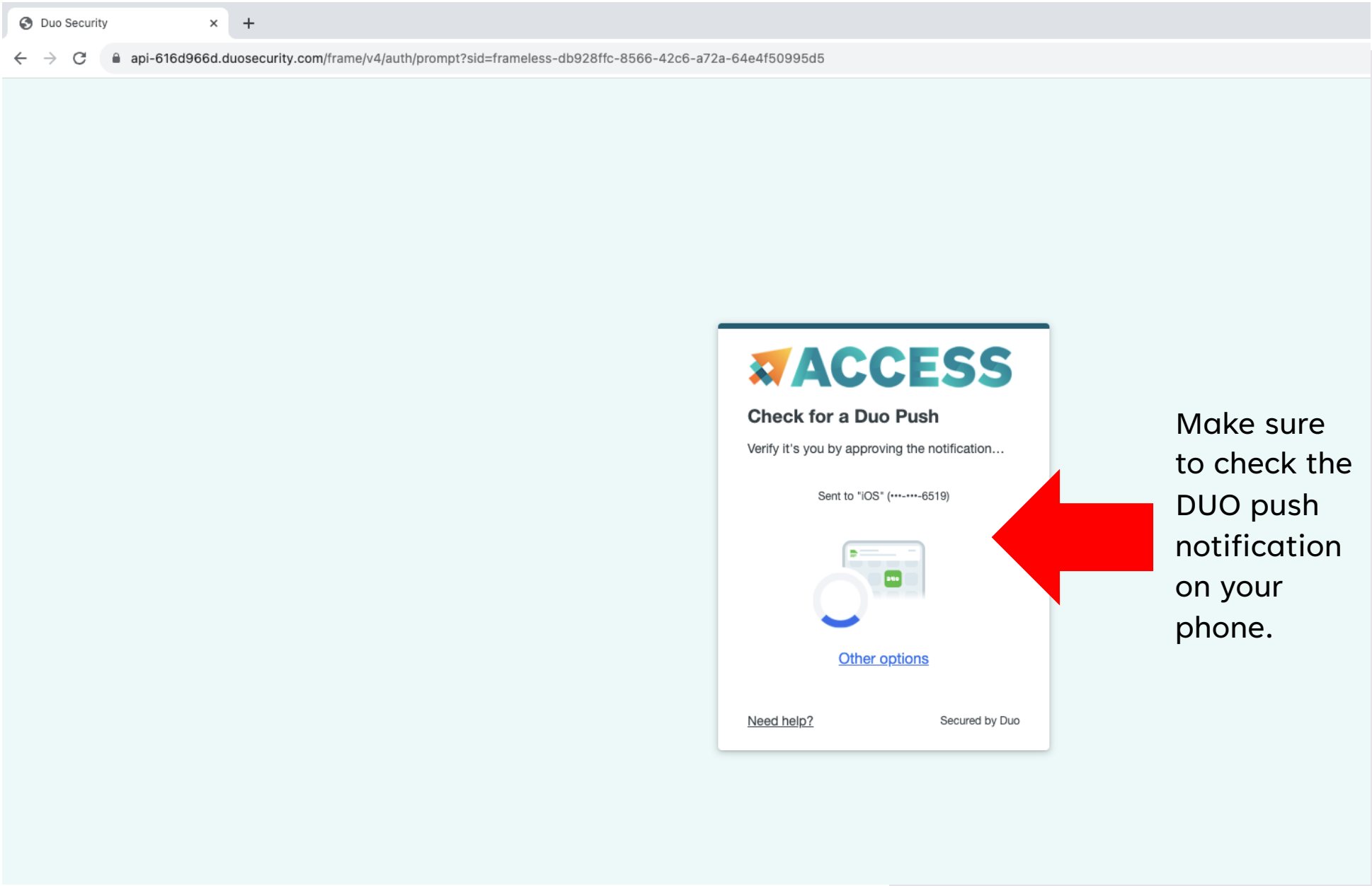
- Make sure to select ACCESS CI (XSEDE) Identity Provider **and NOT CU Anschutz !!!**

Logging into Alpine(5)



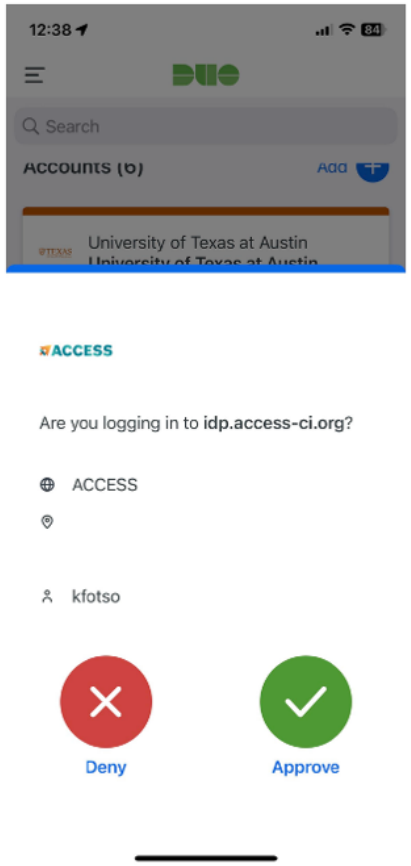
- Enter your **ACCESS** username and password
- Usually, **ACCESS** usernames have the following format: 'firstletteroffirstname ' + 'last name'.

Logging into Alpine(6)



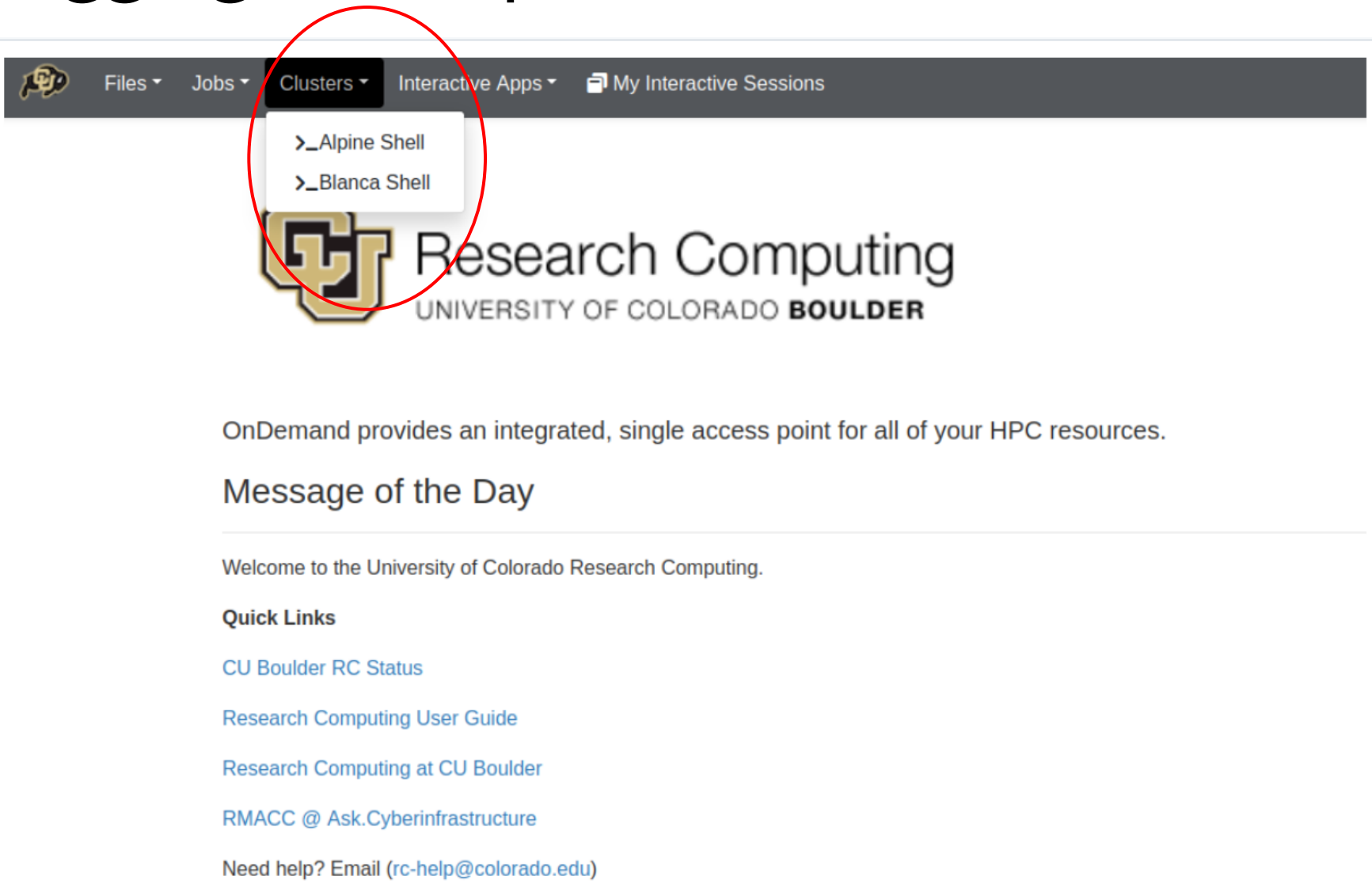
Make sure to check the DUO push notification on your phone.

Logging into Alpine(7)



The authentication confirmation should look similar to the following on your phone.

Logging into Alpine(2)



On the login node (1)

```
Welcome to University of Colorado Boulder Research Computing!

Full documentation is available in our user guide at
https://www.rc.colorado.edu/support/user-guide. If you have a question
that's not answered there, contact us at rc-help@colorado.edu.

A number of directories have been created for you already:

* `/home/$USER`, your home directory
* `/projects/$USER`, your project directory

Run the command `module avail` to see a list of available software.

To prevent this README from being displayed at login, edit your
`.bash_profile` or `.login` files.
bash: /usr/bin/python: No such file or directory
Welcome to CU-Boulder Research Computing.

  * Website http://colorado.edu/rc
  * Questions? rc-help@colorado.edu
  * Subscribe to system announcements: https://curc.statuspage.io/
  * Please type rc-help for the Acceptable Use Policy and a short help page.

You are using login node: login-ci1

bash: /usr/bin/python: No such file or directory
[kfotso@xsede.org@login-ci1 ~]$
```

Name of the username

On the login node (2)

```
Welcome to University of Colorado Boulder Research Computing!

Full documentation is available in our user guide at
https://www.rc.colorado.edu/support/user-guide. If you have a question
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  * Please type rc-help for the Acceptable Use Policy and a short help page.

You are using login node: login-ci1

bash: /usr/bin/python: No such file or directory
[kfotso@xsede.org@login-ci1 ~]$
```

Name of the login node (hostname)

Storage(1)

+

- Home filesystem (2G). Backed up + for hosting config files.
- Project filesystem (250G). Backed up -> for package installation
- “cd .snapshot” to access those back ups
- ‘curc-quota’ or ‘du’ to check on space

Storage(2)

```
[kfotso@xsede.org@login-ci1 ~]$ curc-quota
---------------------------------------------------------------------
                                  Used         Avail    Quota Limit
---------------------------------------------------------------------
/home/kfotso@xsede.org             289M          1.8G          2.0G
/projects/kfotso@xsede.org         144G          107G          250G
/scratch/alpine1                  7786G         20825G         28611G
```

+

Storage(3)

- Scratch space (10 TB)
- GPFS filesystem
- Very suitable for parallel application + heavy I/O
- Purged every 90 days

Petalibrary

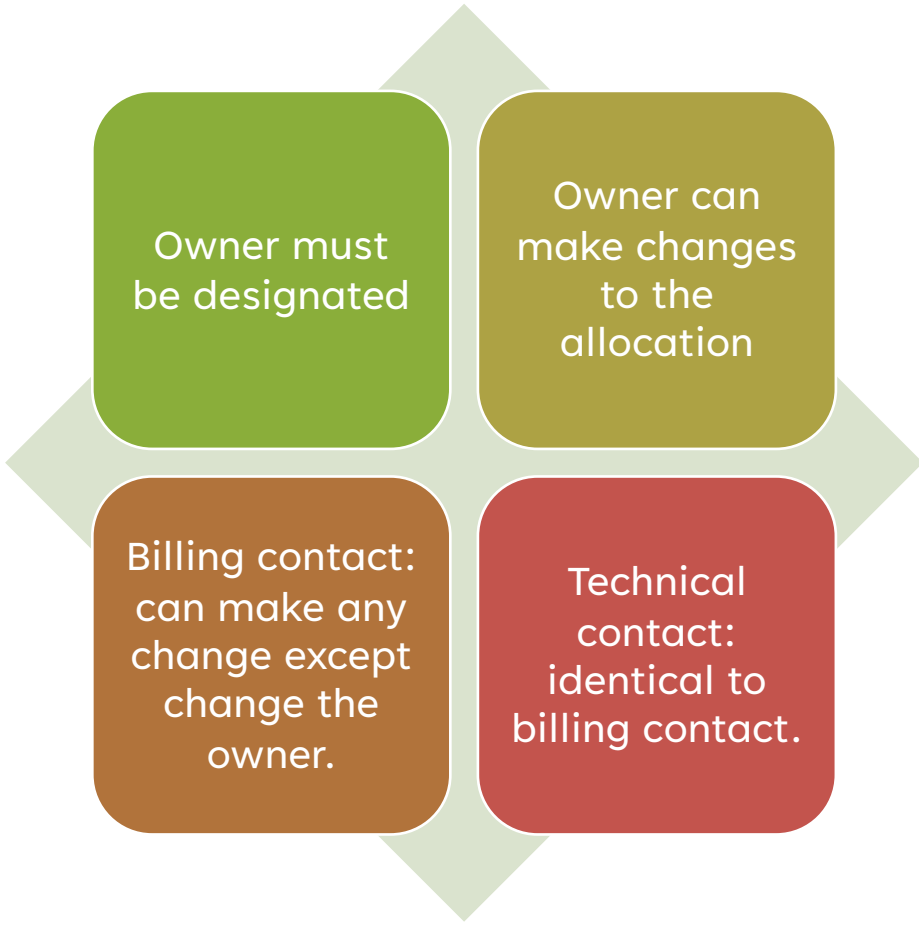
Preliminary conditions (1)

CREATION OF AN ACCESS GROUP

ALL MEMBER ADDED TO THE GROUP WILL NEED ACCESS/XSEDE ACCOUNTS.

```
/pl/active/<your_allocation_name>
/pl/archive/<your_allocation_name>
```

Preliminary conditions (2)



Application

- Application submitted here: https://www.colorado.edu/rc/resources/petalibrary
- The request form will need a speedtype: account# to which they plan to charge the allocation.

Billing (1)

- On active storage: $45/TB/yr.
- ZFS Raidz2 allow for frequent read/write + parity.
- It is highly suggested that total TB size for the year is determined in advanced by the owner.

Billing (2)

- On archive storage: $20/TB/yr.
- Tape-like storage for infrequently accessed data.
- Can be accessed from RC login node only and data transfer resources.
- Min size for any alloc is 1 TB

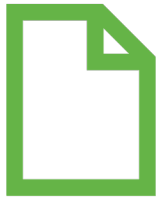
Terms of usage

- Data will need to be in full compliance with term of service.
- No PHI data, no FERPA, no ITAR, no GDPR, no export control and data/software that comply with IRB requirements.
- More information here: https://www.colorado.edu/rc/resources/petalibrary/tos
- Data classification: https://www.cu.edu/security/data-classification.

+

- HIPAA identifiers: https://www.dhcs.ca.gov/dataanddstats/data/Pages/ListofHIPAAIdentifiers.aspx

Data redundancy (1)



PL allocations are of single-copy nature.

All users should fill out the PL single copy acknowledgment.

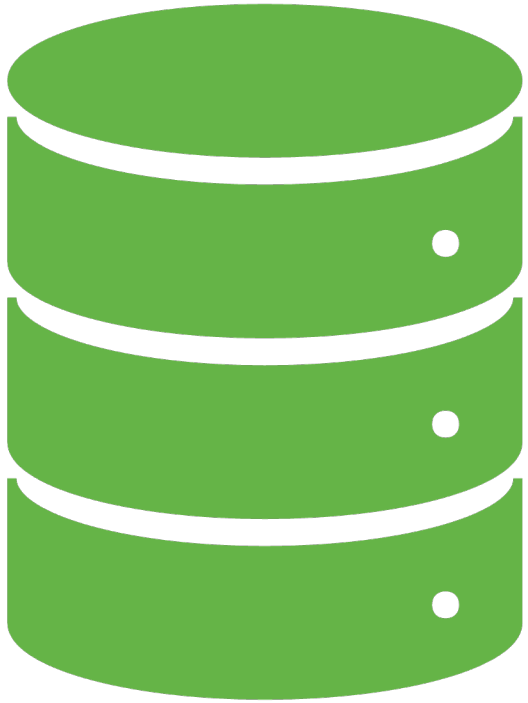
Snapshots monitoring in place so that they are not missed unless on snapshot custom schedule

Sort term back up solutions (1)

- Microsoft OneDrive: 5TB per person through A3 licensing.
- S3 buckets: customer paid & rates located here: https://aws.amazon.com/s3/pricing/?p=pm&c=s3&z=4
- Multiple PL allocations as though customer requested 2 allocations (X2 price).

Sort+mid term back up solutions (2)

- [BETA]
  Replicated PetaLibrary active +archive allocation.
- Nothing is charged during beta period but will likely look like Multiple PL allocations.
- CURC only takes data replication responsibility for BETA



Active+Archive replication

- Synchronization between active and archive happen every 15 min in theory but are not always guaranteed.
- Snapshots are also replicated from active to archive.
- The Boulder storage team maintains the second copy (e.g. archive) for you and you do not have direct access to it.
- $65/TB/year total. **(NOT $65 on top of the $45/$20 original rate!!)**

Files transfer (Globus)

1

Creation of Globus Connect Personal endpoint.

2

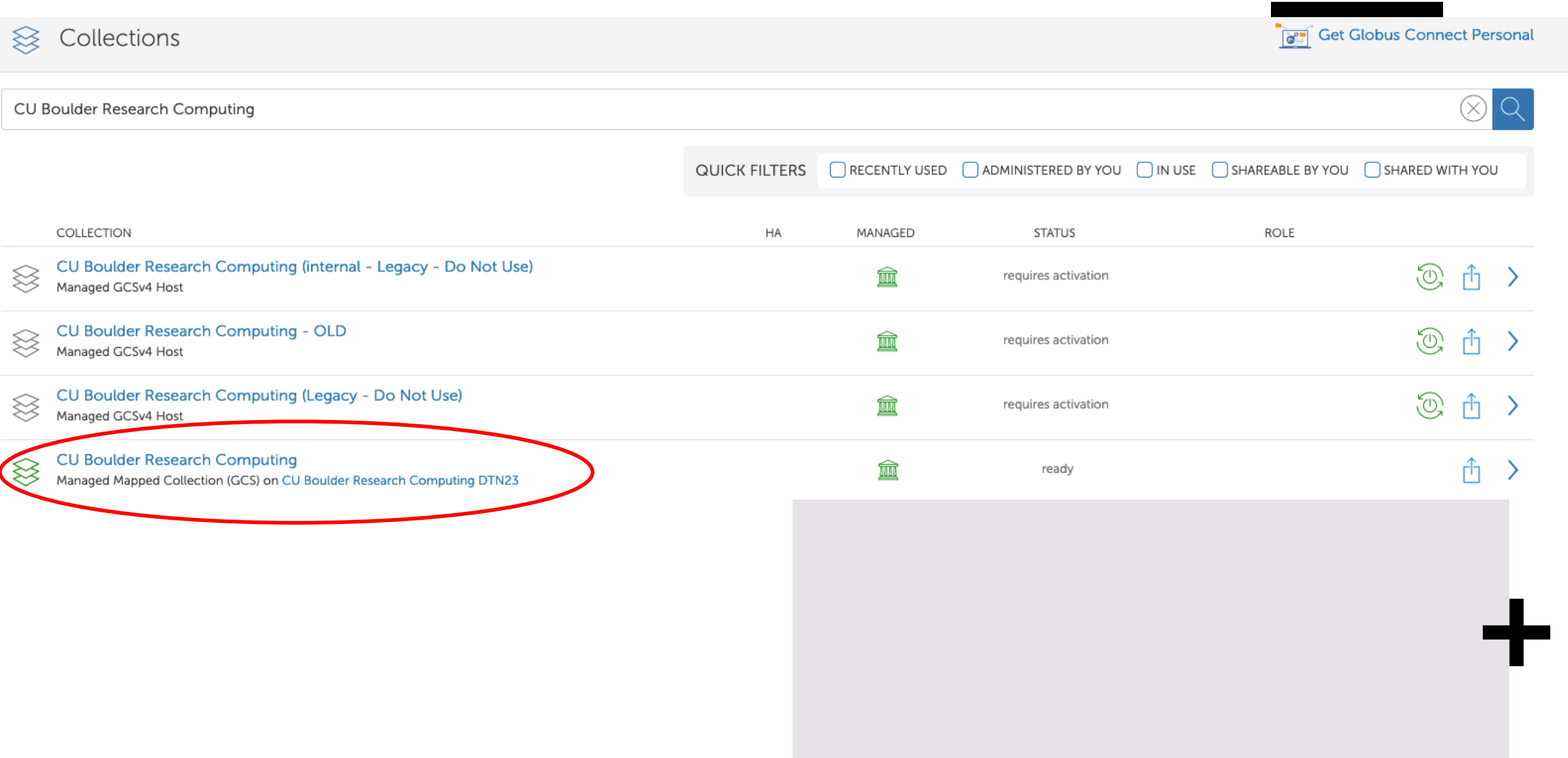
CU Boulder endpoint for Anschutz was CU Boulder Research Computing ACCESS.

3

Current ACCESS point (DTN23) is 10X faster than the legacy one

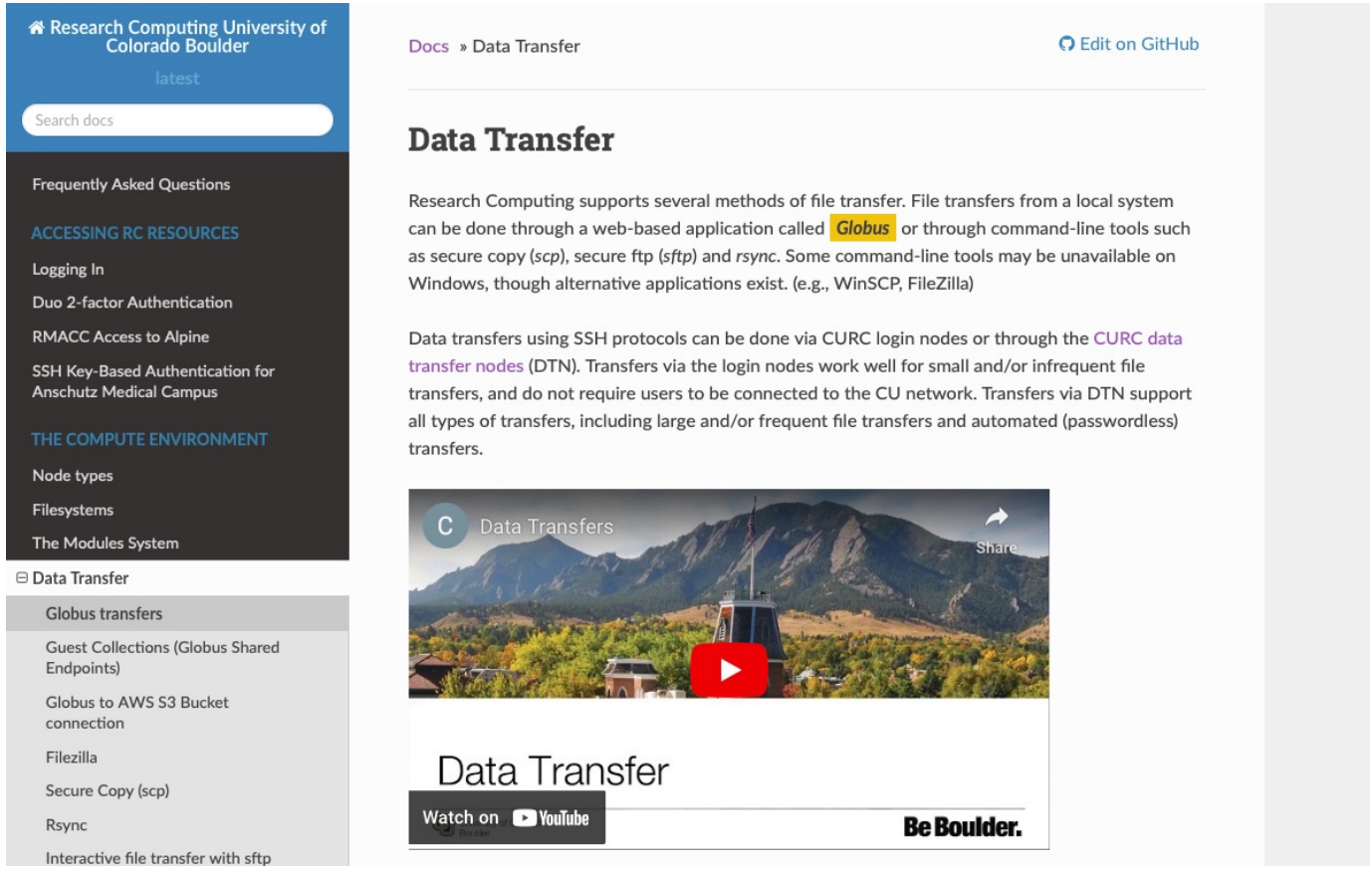
“CU Boulder Research Computing”

Globus (2)


Collections
Get Globus Connect Personal
CU Boulder Research Computing
QUICK FILTERS
RECENTLY USED
ADMINISTERED BY YOU
IN USE
SHAREABLE BY YOU
SHARED WITH YOU
COLLECTION
HA
MANAGED
STATUS
ROLE
CU Boulder Research Computing (internal - Legacy - Do Not Use)
Managed GCSv4 Host
requires activation
CU Boulder Research Computing - OLD
Managed GCSv4 Host
requires activation
CU Boulder Research Computing (Legacy - Do Not Use)
Managed GCSv4 Host
requires activation
CU Boulder Research Computing
Managed Mapped Collection (GCS) on CU Boulder Research Computing DTN23
ready

Globus(3)

- More info here: https://curc.readthedocs.io/en/latest/compute/data-transfer.html?highlight=globus#globus-transfers



II) - Alpine computing

Scheduler Slurm

acompile --ntasks=1 --time=00:30:00 to build packages and do some testing. (max 12 hours)

sinteractive --ntasks-per-node=2 --nodes=2

--partition=atesting to test pipelines. (max 1 hour)

```
[kfotso@xsede.org@login-ci1 kfotso@xsede.org]$ sinfo --partition=aa100
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
aa100        up 1-00:00:00      1   resv c3gpu-a9-u33-1
aa100        up 1-00:00:00      7    mix c3gpu-a9-u31-1,c3gpu-a9-u35-1,c3gpu-c2-u
aa100        up 1-00:00:00      4  alloc c3gpu-a9-u29-1,c3gpu-c2-u[7,13,15]
```

sinfo

Can be used to get information about a node.

Package availability (1)

Some packages that have been built and accessible through lmod.

Adding new packages through lmod takes a lot of round of approval so it is recommended to build them locally.

Solutions: (cmake+make), Anaconda, pip, containers, spack etc ...

Submit a ticket at rc-help@Colorado.edu so that I can build it for you locally.

LMOD (CONTEXT)

- Modern environment module system for HPC
- Initially introduced by Robert McLay from TACC (UT Austin) in 2011.

LMOD (CONTEXT)

- Users have on HPC have different needs.

- Applications, compilers, libraries, versions being used might be different.

LMOD (benefits)

- Users do not need to know where software is installed
- Environment variable to interface packages can be set (e.g. picard).
- Very useful for software reproducibility

LMOD (benefits)

- Supports software hierarchy
- Users can set their environment modules at will.

List of officially available bio modules

- “acompile”
- “module avail”

```
   alphafold/2.2.0          bcftools/1.16       cellranger/7.1.0
   alphafold/2.3.1 (D)      bedtools/2.29.1     cutadapt/4.2
   bamtools/2.5.2           bowtie2/2.5.0       fastqc/0.11.9
   bbtools/39.01            bwa/0.7.17          gatk/4.3.0.0
```

```
htslib/1.16                 picard/2.27.5       sra-toolkit/3.0.0
multiqc/1.14                plink2/2.00a2.3     star/2.7.10b
nextflow/22.10.6            qiime2/2023.5       trimmomatic/0.39
nextflow/23.04    (D)       samtools/1.16.1
```

Slurm example

```
#!/bin/bash

#SBATCH --partition=amilan
#SBATCH --job-name=example-job
#SBATCH --output=example-job.%j.out
#SBATCH --time=01:00:00
#SBATCH --qos=normal
#SBATCH --nodes=1
#SBATCH --ntasks=4
#SBATCH --mail-type=ALL
#SBATCH --mail-user=youridentikey@colorado.edu

module purge
module load anaconda
conda activate custom-env

python myscript.py
```

Your shell is bash

Partition is amilan (CPU)

Job name when it gets queued

Output file name

How long my job runs?

Slurm example

```
#!/bin/bash

#SBATCH --partition=amilan
#SBATCH --job-name=example-job
#SBATCH --output=example-job.%j.out
#SBATCH --time=01:00:00
#SBATCH --qos=normal
#SBATCH --nodes=1
#SBATCH --ntasks=4
#SBATCH --mail-type=ALL
#SBATCH --mail-user=youridentikey@colorado.edu

module purge
module load anaconda
conda activate custom-env

python myscript.py
```

Quality of service

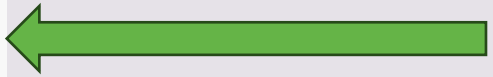
How many nodes I want to run on?

Slurm example

```
#!/bin/bash

#SBATCH --partition=amilan
#SBATCH --job-name=example-job
#SBATCH --output=example-job.%j.out
#SBATCH --time=01:00:00
#SBATCH --qos=normal
#SBATCH --nodes=1
#SBATCH --ntasks=4
#SBATCH --mail-type=ALL
#SBATCH --mail-user=youridentikey@colorado.edu

module purge
module load anaconda
conda activate custom-env

python myscript.py
```

Total cores used

Email when job begins, ends and fails



Email address

Slurm example

```
#!/bin/bash

#SBATCH --partition=amilan
#SBATCH --job-name=example-job
#SBATCH --output=example-job.%j.out
#SBATCH --time=01:00:00
#SBATCH --qos=normal
#SBATCH --nodes=1
#SBATCH --ntasks=4
#SBATCH --mail-type=ALL
#SBATCH --mail-user=youridentikey@colorado.edu

module purge
module load anaconda
conda activate custom-env

python myscript.py
```

Reinitialize module list

Load anaconda

Activate environment

Running pipeline command

Slurm cheatsheet (1)

Slurm script command	Description
#!/bin/bash	Sets the shell that the job will be executed on the compute node
#SBATCH --ntasks=1 #SBATCH --n1	Requests for 1 processors on task, usually 1 cpu as 1 cpu per task is default.
#SBATCH --time=0-05:00 #SBATCH -t 0-05:00	Sets the maximum runtime of 5 hours for your job
#SBATCH --mail-user= <email>	Sets the email address for sending notifications about your job state.
#SBATCH --mail-type=BEGIN #SBATCH --mail-type=END #SBATCH --mail-type=FAIL #SBATCH --mail-type=REQUEUE #SBATCH --mail-type=ALL	Sets the scedualing system to send you email when the job enters the follwoing states: BEGIN,END,FAIL,REQUEUE,ALL
#SBATCH --job-name=my-named-job	Sets the Jobs name

Slurm cheatsheet(2)

Slurm script command	Description
#SBATCH −ntasks=X	Requests for X tasks. When cpus-per-task=1 (and this is the default) this requests X cores. When not otherwise constraint these CPUs may be running on any node
#SBATCH --nodes=X	Request that a minimum of X nodes be allocated to this job
#SBATCH --nodes=X-Y	Request that a minimum of X nodes and a maximum of Y nodes be allocated to this job
#SBATCH --cpus-per-task=X	Request that a minimum of X CPUs per task be allocated to this job
#SBATCH --tasks-per-node=X	Requests minimum of X task be allocated per node

Slurm cheatsheet(3)

Slurm script commands	Description of effects
#SBATCH --ntasks=1 #SBATCH --cpus-per-task=1	Requests 1 CPU (Serial) cpus-per-task is set to 1 by default and may be omitted.
#SBATCH --cpus-per-task=X #SBATCH --ntasks=1 #SBATCH --nodes=1	Requests for X CPUs in 1 task on 1 node (OpenMP) Both ntasks and nodes are set to 1 by default and may be omitted
#SBATCH --ntasks=X #SBATCH --tasks-per-node=X #SBATCH --cpus-per-task=1	Requests for X CPUs and tasks on 1 node cpus-per-task is set to 1 by default and may be omitted.
#SBATCH --ntasks=X #SBATCH --nodes=1 #SBATCH --cpus-per-task=1	Requests for X CPUs and tasks on 1 node cpus-per-task is set to 1 by default and may be omitted.

Get information about jobs

```
[kfotso@xsede.org@login-ci1 ~]$ squeue -l --me
  JOBID PARTITION     NAME     USER    STATE       TIME TIME_LIMI  NODES NODELIST(REASON)
2158225  acompile acompile kfotso@x  RUNNING       0:16      3:00      1 c3cpu-c11-u21-2
```

Monitor resources

```
[kfotso@xsede.org@login-ci1 ~]$ module load slurmtools
[kfotso@xsede.org@login-ci1 ~]$ jobstats $USER 2
job stats for user kfotso@xsede.org over past 2 days
jobid        jobname  partition    qos          account      cpus state    start-date-time     elapsed    wait
-------------------------------------------------------------------------------------------------------------
2064187      sinterac atesting_+   testing      amc-gener+   48   TIMEOUT  2023-06-20T23:32:52 01:00:04   0 hrs
2071952      vep_loft aa100        normal       amc-gener+   64   COMPLETE 2023-06-21T13:47:55 00:26:42   3 hrs
```

- Allows to get information about a past jobs

```
[kfotso@xsede.org@login-ci1 ~]$ seff 1451164
Job ID: 1451164
Cluster: alpine
User/Group: kfotso@xsede.org/kfotsopgrp@xsede.org
State: COMPLETED (exit code 0)
Nodes: 1
Cores per node: 48
CPU Utilized: 26-03:21:39
CPU Efficiency: 94.06% of 27-19:00:48 core-walltime
Job Wall-clock time: 13:53:46
Memory Utilized: 412.77 GB
Memory Efficiency: 41.28% of 999.98 GB
```

- To get more computational information about the job efficiency

Slurm Quality of service (qos)

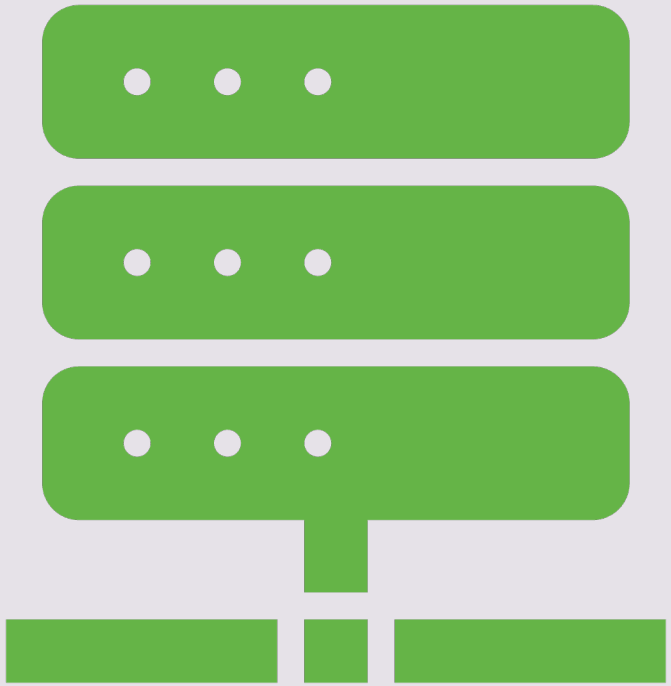
- Used to modify or constrain characteristics that a job can have.
- **--qos=normal** corresponds to a walltime of 24 hours and is the default.
- **--qos=long** corresponds to a walltime of up to 7 days
- **--qos=mem** corresponds to high memory jobs only (up to 1TB)

Fairshare overview

- Difference between the portion of computing resource that has been promised and the amount of resources that has been consumed.

- Level fairshare of 1 indicates average priority compared to other users in that account (amc-general)

- **module load slurmtools; levelfs $USER**



Job priority calculation formula

```
Job_priority =
        site_factor +
        (PriorityWeightAge) * (age_factor) +
        (PriorityWeightAssoc) * (assoc_factor) +
        (PriorityWeightFairshare) * (fair-share_factor) +
        (PriorityWeightJobSize) * (job_size_factor) +
        (PriorityWeightPartition) * (partition_factor) +
        (PriorityWeightQOS) * (QOS_factor) +
        SUM(TRES_weight_cpu * TRES_factor_cpu,
            TRES_weight_<type> * TRES_factor_<type>,
            ...)
        - nice_factor
```

Check fairshare

```
Host: login-ci1.rc.int.colorado.edu
[kfotso@xsede.org@login-ci1 ~]$ levelfs $USER

LevelFS for user kfotso@xsede.org and institution amc:

Account              LevelFS_User         LevelFS_Inst
---------------------------------------------------------
amc-general          0.194275             4.750220
[kfotso@xsede.org@login-ci1 ~]$
```

- 0.19 means that my priority will be low
- On the other hand 4.75 means that priority for the institution is high

Service Units (SU)

– It is the number of core hours used.

```
[kfotso@xsede.org@login-ci1 ~]$ suuser $USER 10
SU used by user kfotso@xsede.org in the last 10 days:
Cluster|Account|Login|Proper Name|TRES Name|Used|
alpine|amc-general|kfotso@xsede.org|Kevin Fotso|billing|8393|
```

– suacct to get the number of core hours used by institution

```
Host: login-ci1.rc.int.colorado.edu
[kfotso@xsede.org@login-ci1 ~]$ suacct amc-general 180
SU used by account (allocation) amc-general in the last 180 days:
Cluster|Account|Login|Proper Name|TRES Name|Used
alpine|amc-general|||billing|1806360
alpine| amc-general|acozart@xsede.org|Abigail Cozart|billing|573
alpine| amc-general|agillen@xsede.org|Austin Gillen|billing|40320
alpine| amc-general|agray@xsede.org|Alyx Gray|billing|22
```

Best practices on Alpine (1)

– /home or /tmp have a very small size. Please always include the following in your slurm script.

```
export TMP=/scratch/alpine/$USER
export TEMP=/scratch/alpine/$USER
export TMPDIR=/scratch/alpine/$USER
export TEMPDIR=/scratch/alpine/$USER
```

Best practices on Alpine (2)

– /home or /tmp have a very small size. Please always include the following in your slurm script.

export TMP=/scratch/alpine/$USER

export TEMP=/scratch/alpine/$USER

export TMPDIR=/scratch/alpine/$USER

export TEMPDIR=/scratch/alpine/$USER

-In general, always make sure to check your .cache in $HOME to make sure you are not running out of space.

Best practices on Alpine (3) - Username Aliasing

- /home/foo@xsede.org/ → /home/.xsede.org/foo/
- /projects/foo@xsede.org -> /projects/.xsede.org/foo/
- /scratch/alpine/foo@xsede.org -> /scratch/alpine/.xsede.org/foo/

Best practices on Alpine (4) – Anaconda config

– Edit the .condarc file located in $HOME/.condarc with the editor of choice (e.g. nano, vim etc ...)

– Paste the following 4 lines in the file and exit.

```
pkgs_dirs:
    - /projects/.xsede.org/foo/.conda_pkgs
envs_dirs:
    - /projects/.xsede.org/foo/software/anaconda/envs
```

Brief mention of parallelism

- OpenMP (multithreading).
- MPI (Parallel distribution between multiple nodes)
- GNU parallel (embarrassingly parallel)
- Job arrays (max 1000 on Alpine)
- Load balancing (developed by CU Boulder)
- GPU computing

Slurm example to see the number of cores(1)

- Here, we are requesting 4 cores for a 2 minutes

```
[kfotso@xsede.org@login-ci2 ~]$ acompile --ntasks=4 --time=00:02:00
acompile: submitting job... salloc --nodes=1 --partition=acompile --ntasks=4  --time=00:02:00  --qos=compile --job-name=acompile --bell
--oversubscribe srun --pty /bin/bash
salloc: Granted job allocation 2998293
salloc: Nodes c3cpu-a5-u32-1 are ready for job
```

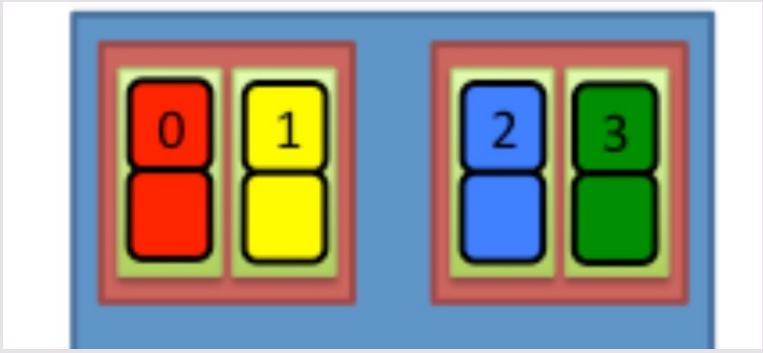
- We are getting node c3cpu-a5-u32-1 and our jobID is 2998293

Slurm example to see the number of cores(2)

- We want load compiler gcc because openmpi depends on it

```
[kfotso@xsede.org@c3cpu-a5-u32-1 ~]$ module load gcc
[kfotso@xsede.org@c3cpu-a5-u32-1 ~]$ module load openmpi
```

- We want to use openmpi because we want to demonstrate parallelism on the 4 cores we have reserved



Slurm example to see the number of cores(3)

- hostname is just a program that prints the name of the node I am working with

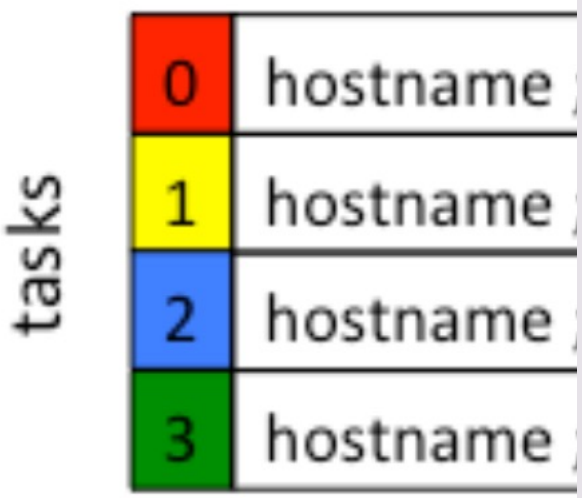
```
[kfotso@xsede.org@c3cpu-a5-u32-1 ~]$ mpirun -n 4 hostname
c3cpu-a5-u32-1.rc.int.colorado.edu
c3cpu-a5-u32-1.rc.int.colorado.edu
c3cpu-a5-u32-1.rc.int.colorado.edu
c3cpu-a5-u32-1.rc.int.colorado.edu
```

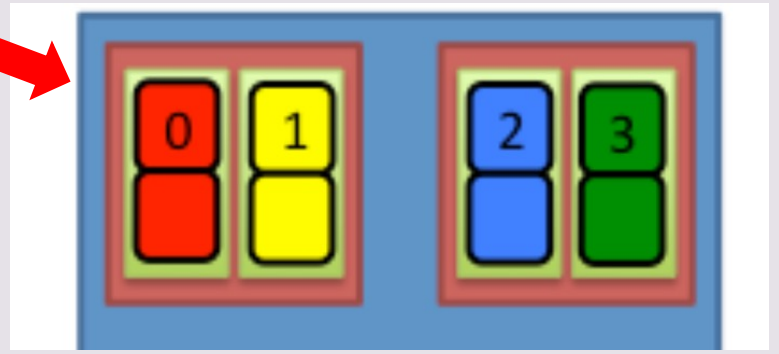
- With mpirun, we schedule 4 tasks on the 4 cores, thus the name of the name of the node gets printed 4 times !!!

Slurm example to see the number of cores(4)

Recap of what we did

mpirun –n 4 hostname

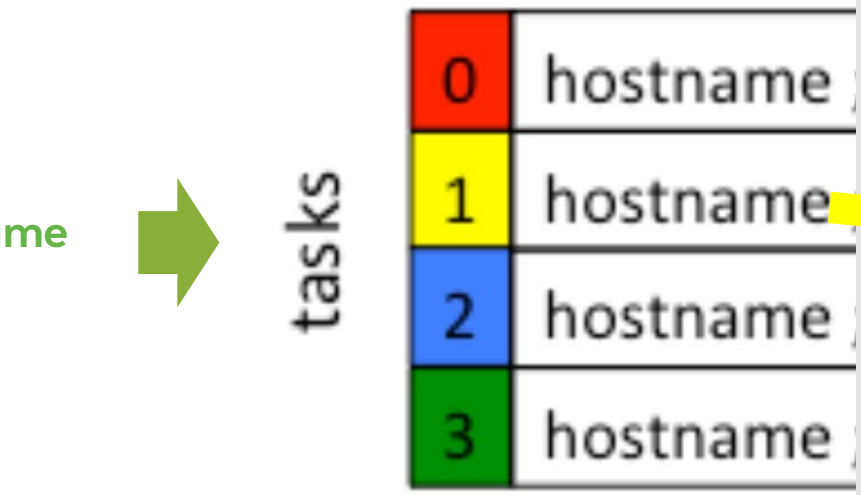


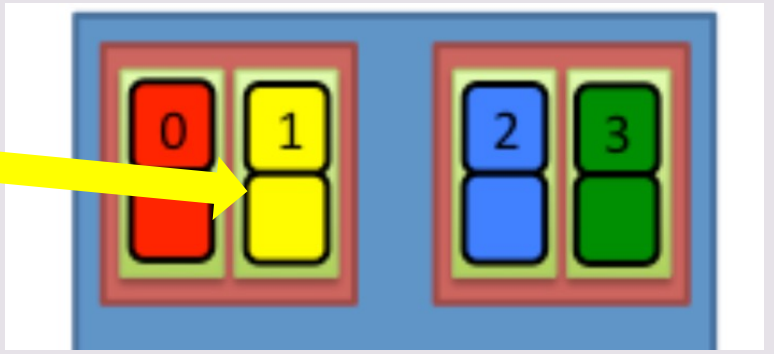


Slurm example to see the number of cores(4)

Recap of what we did

mpirun –n 4 hostname

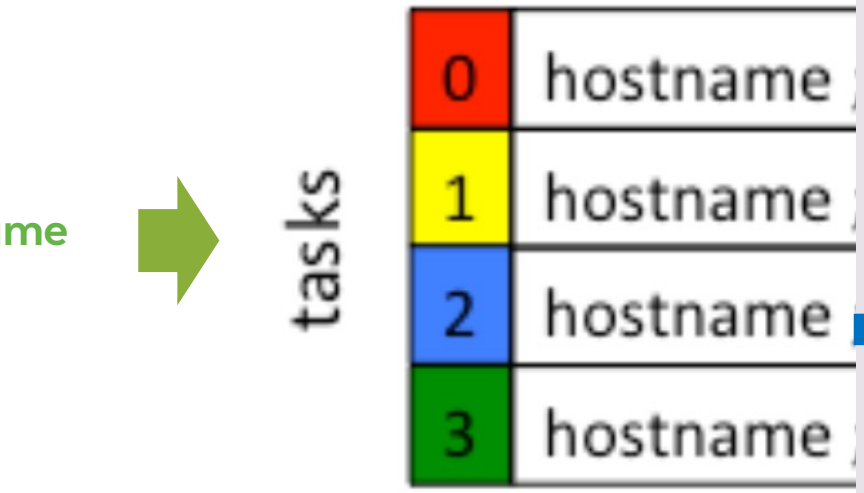


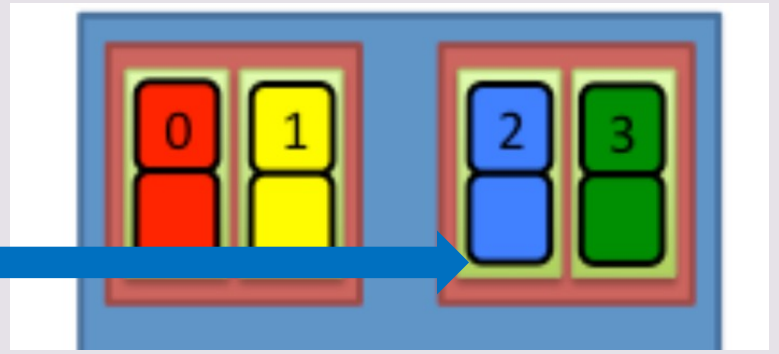


Slurm example to see the number of cores(4)

Recap of what we did

mpirun –n 4 hostname

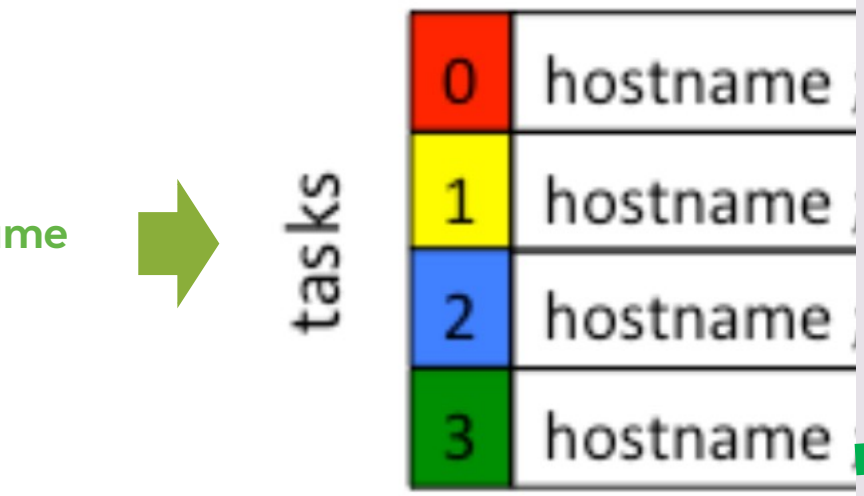


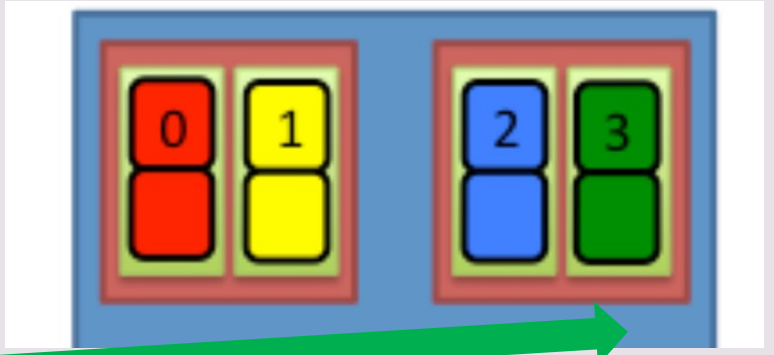


Slurm example to see the number of cores(4)

Recap of what we did

mpirun –n 4 hostname

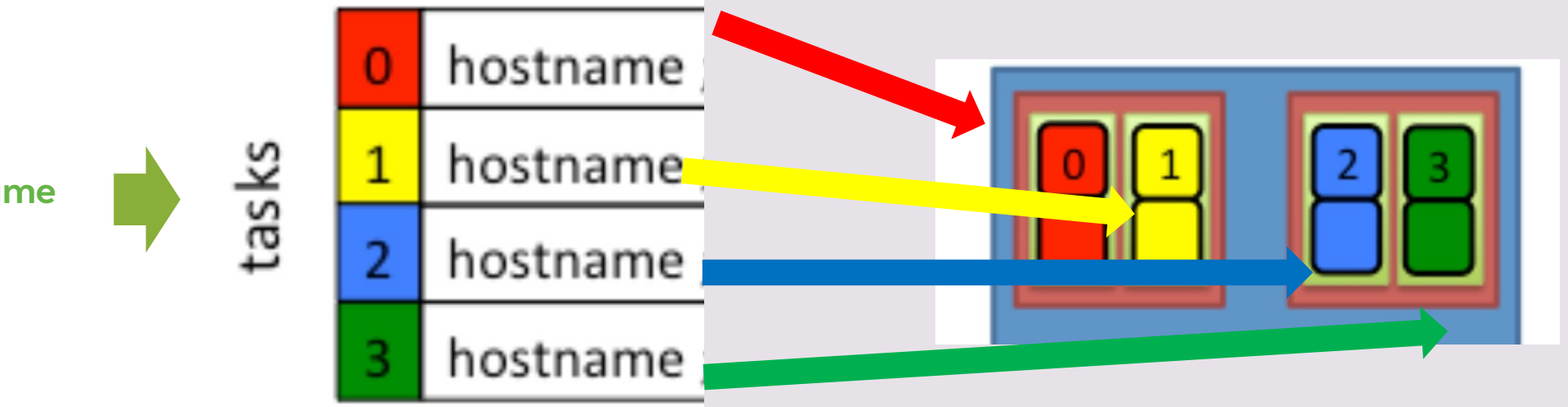




Slurm example to see the number of cores(4)

Recap of what we did

mpirun –n 4 hostname



Slurm example to see the number of cores(5)

– Congratulations!!! You just wrote your first HPC parallel code program!

Build the corresponding slurm script (1)

- Create the empty slurm script and modify it with your editor of choice (nano, vim, emac, Ondemand etc ...)

```
[kfotso@xsede.org@login-ci2 openmpi_hostname]$ touch hello_mpi.sh
[kfotso@xsede.org@login-ci2 openmpi_hostname]$
```

Build the corresponding slurm script

```
#!/bin/bash

#SBATCH --partition=amilan
#SBATCH --job-name=first_mpirun
#SBATCH --output=first_mpirun-job.%j.out
#SBATCH --error=first_mpirun-job.%j.err
#SBATCH --account=amc-general
#SBATCH --qos=normal
#SBATCH --nodes=1
#SBATCH --ntasks=4
#SBATCH --mail-type=ALL
#SBATCH --mail-user=kfotsotagne@unm.edu
#SBATCH --time=00:00:01

module load gcc
module load openmpi

mpirun -n $SLURM_NTASKS hostname
```

Account name is amc-general

Job runs for 1 second!!

Build the corresponding slurm script

```
#!/bin/bash

#SBATCH --partition=amilan
#SBATCH --job-name=first_mpirun
#SBATCH --output=first_mpirun-job.%j.out
#SBATCH --error=first_mpirun-job.%j.err
#SBATCH --account=amc-general
#SBATCH --qos=normal
#SBATCH --nodes=1
#SBATCH --ntasks=4
#SBATCH --mail-type=ALL
#SBATCH --mail-user=kfotsotagne@unm.edu
#SBATCH --time=00:00:01

module load gcc
module load openmpi

mpirun -n $SLURM_NTASKS hostname
```

$SLURM_NTAKS is the slurm env variable for the 4 cores

Build the corresponding slurm script (4)

We use sbatch to submit the script

```
[kfotso@xsede.org@login-ci2 openmpi_hostname]$ sbatch hello_mpi.sh
Submitted batch job 2998325
```

Build the corresponding slurm script (5)

The .out file shows the name of the nodes 4X.

.err file is empty so no error.

```
[kfotso@xsede.org@login-ci2 openmpi_hostname]$ ls -latr
total 184
drwxrws---. 44 kfotso@xsede.org kfotsogrp@xsede.org 1672 Sep 15 01:45 ..
-rw-r--r--.  1 kfotso@xsede.org kfotsogrp@xsede.org  400 Sep 15 01:52 hello_mpi.sh
-rw-r--r--.  1 kfotso@xsede.org kfotsogrp@xsede.org    0 Sep 15 01:52 first_mpirun-job.2998325.err
drwxr-sr-x.  2 kfotso@xsede.org kfotsogrp@xsede.org  122 Sep 15 01:52 .
-rw-r--r--.  1 kfotso@xsede.org kfotsogrp@xsede.org  140 Sep 15 01:52 first_mpirun-job.2998325.out
[kfotso@xsede.org@login-ci2 openmpi_hostname]$ cat first_mpirun-job.2998325.out
c3cpu-c15-u1-2.rc.int.colorado.edu
c3cpu-c15-u1-2.rc.int.colorado.edu
c3cpu-c15-u1-2.rc.int.colorado.edu
c3cpu-c15-u1-2.rc.int.colorado.edu
[kfotso@xsede.org@login-ci2 openmpi_hostname]$
```

Ondemand MATLAB

RC will conduct its monthly planned maintenance on Wednesday, September 6. Please visit curc.statuspage.io for details.

Notice: Users will be limited to a maximum of 8 cores per Core Desktop session through mid-September due to ongoing maintenance.

Home / My Interactive Sessions / MATLAB (Presets)

Interactive Apps

Desktops

- Core Desktop (Presets)

GUIs

- MATLAB (Presets)

Servers

- Jupyter Session (Custom)
- Jupyter Session (Presets)
- RStudio Server (Custom)
- RStudio Server (Presets)
- VS Code-Server (Custom)
- VS Code-Server (Presets)

MATLAB (Presets)

This app will launch a MATLAB GUI on a CURC node. You will be able to interact with MATLAB through a VNC session. GPU based options are not meant for computationally intensive workflows. Additionally, please keep in mind that these GPU based options are a shared resource amongst all users. Thus, significant computation by one user can affect other users of this service.

MATLAB version

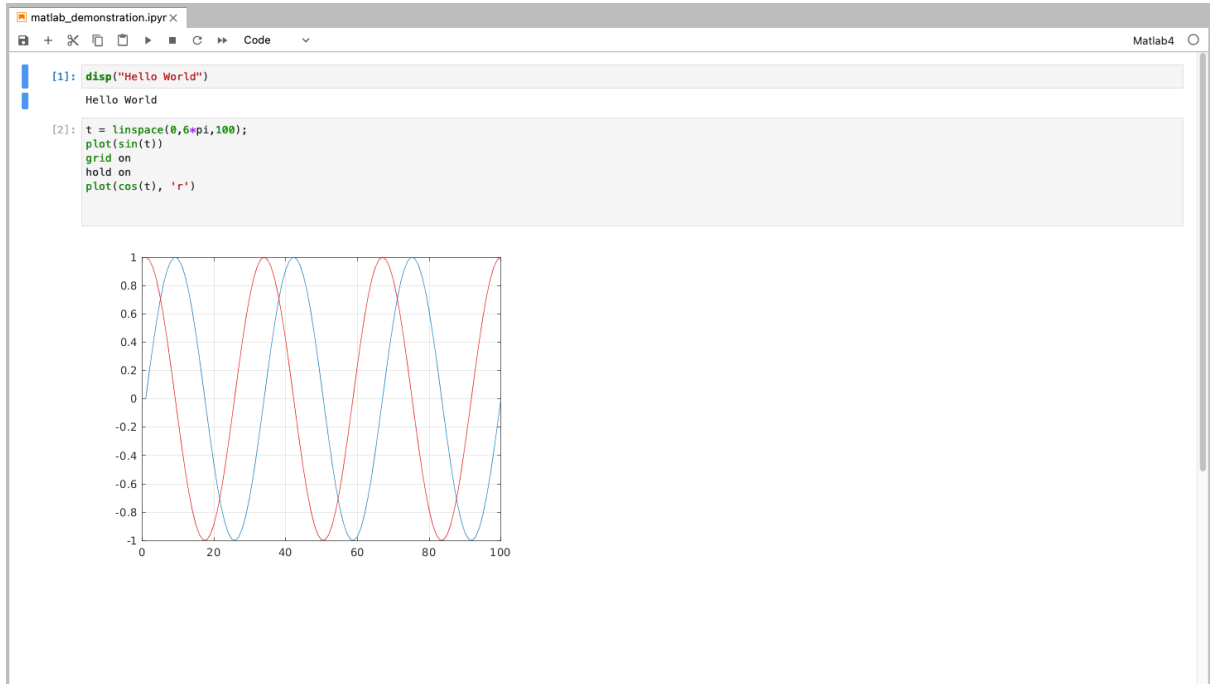
R2021b

Configuration

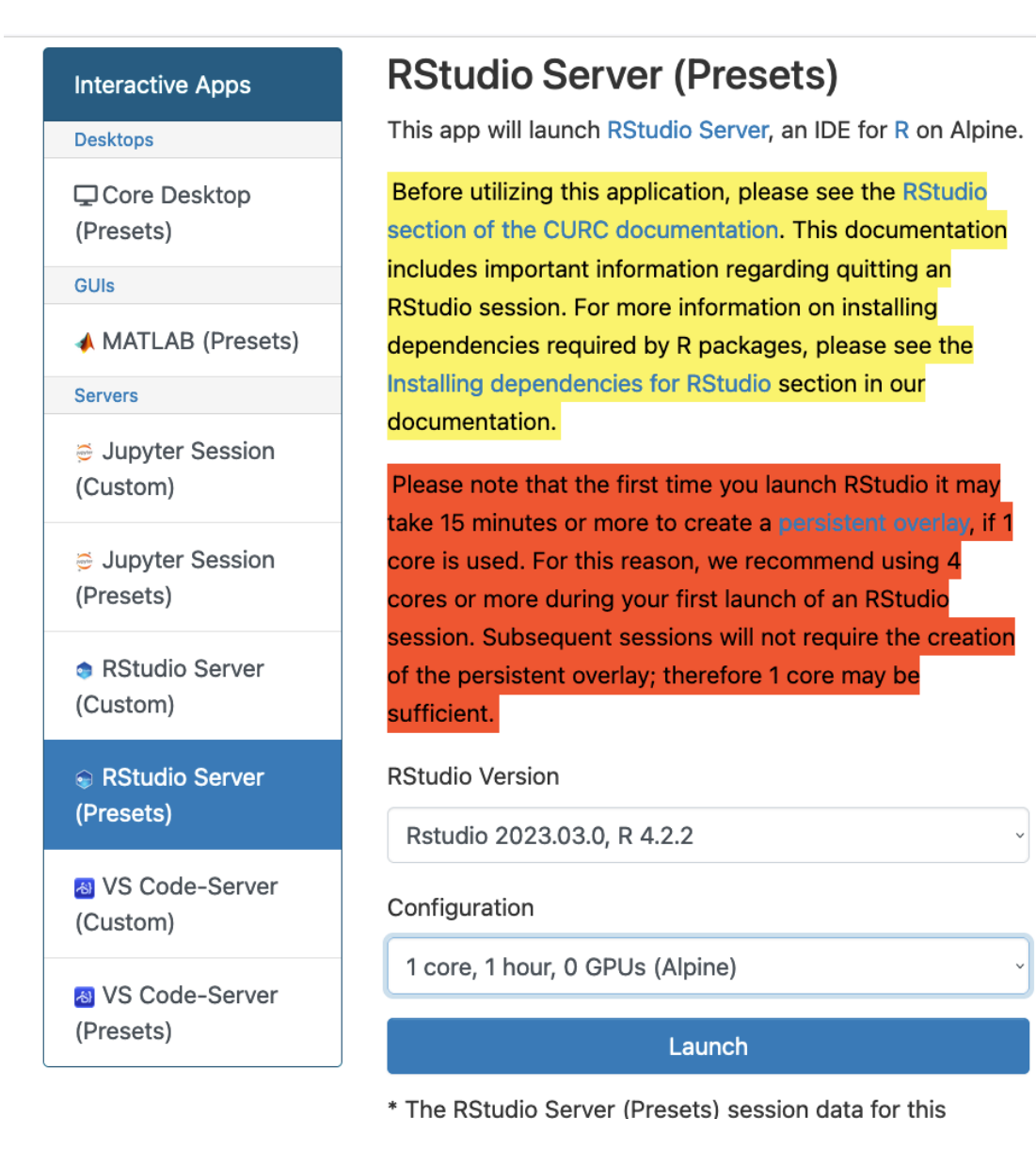
- ✓ 2 cores, 1 hour, K80 GPU
- 2 cores, 1 hour, RTX8000 GPU
- 2 cores, 12 hours, K80 GPU
- 2 cores, 12 hours, RTX8000 GPU
- 4 cores, 4 hours, K80 GPU
- 4 cores, 4 hours, RTX8000 GPU

Ondemand Jupyterlab with MATLAB kernel

- Instructions here: https://github.com/kf-cuanschutz/CU-Anschutz-HPC-documentation/blob/main/MATLAB-kernel-on-Jupyterlab.md
- Possibility to use MATLAB with ssh (if registered)
- MATLAB Ondemand coming soon.

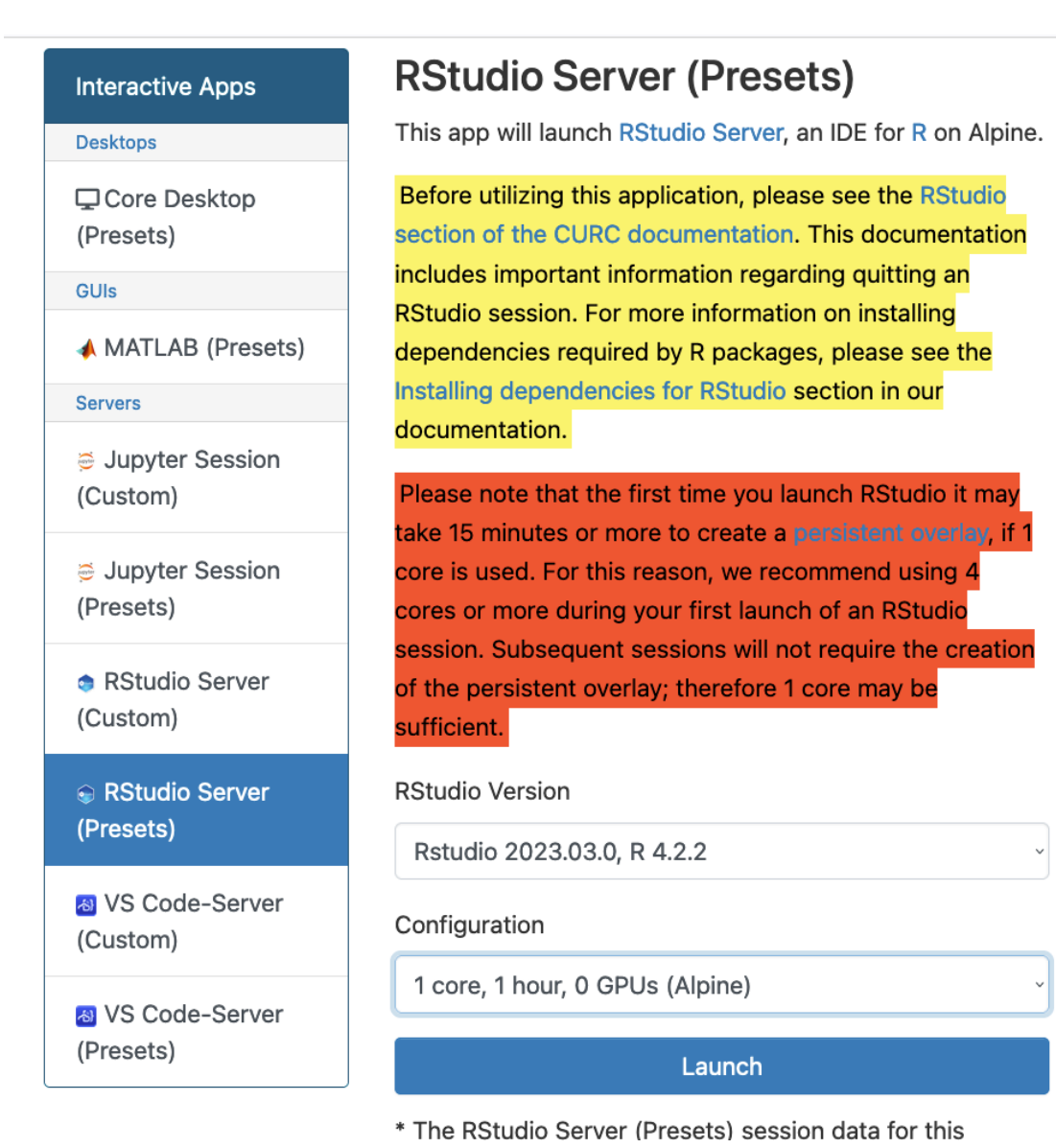


Rstudio with Ondemand (preset)



Important: It already interact with the Slurm scheduler!!!

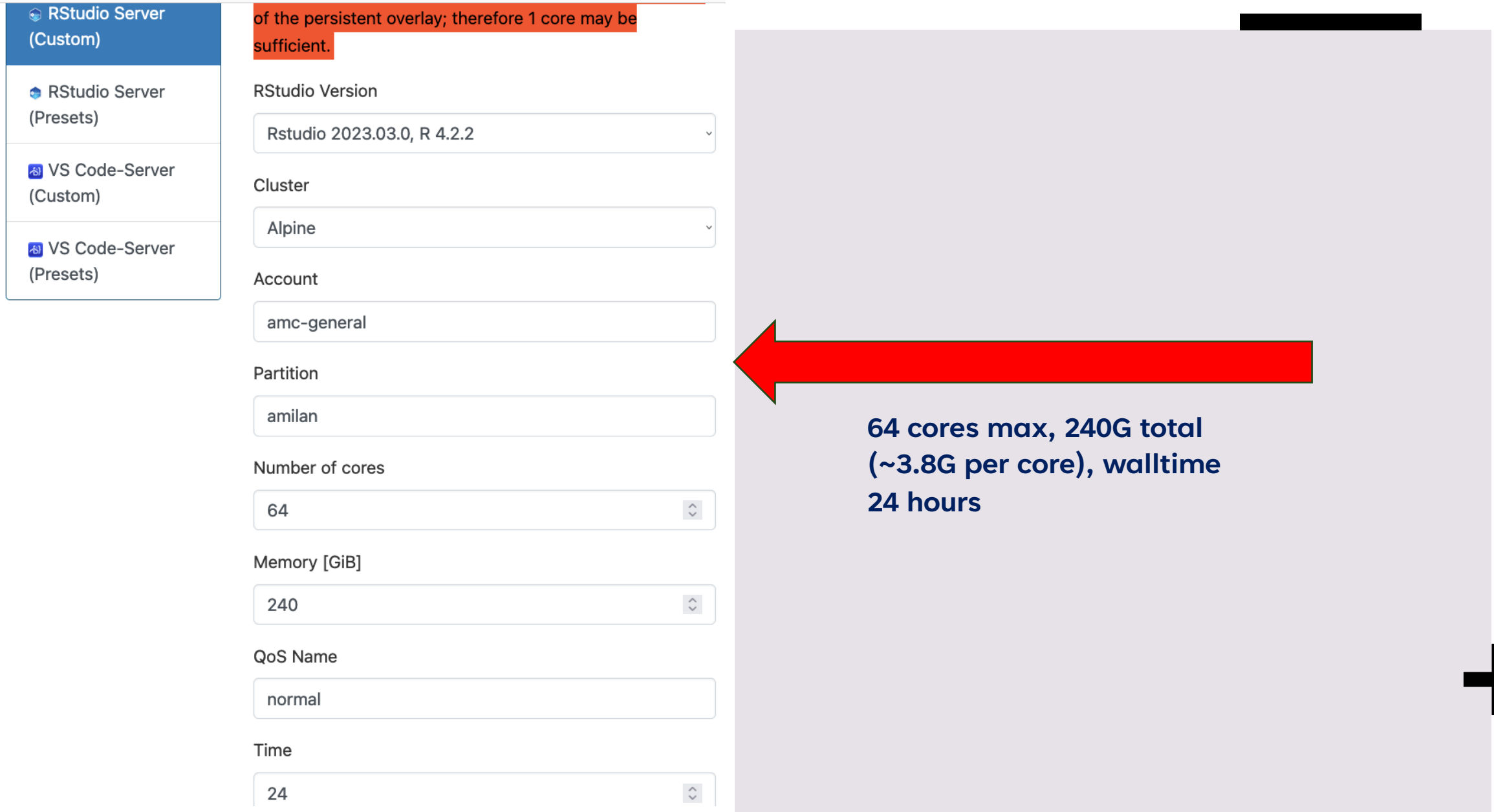
Rstudio with Ondemand (preset)



Important: It already interact with the Slurm scheduler!!!

Preset option comes with already set parameters (e.g. 1 core or 4 cores)

Rstudio with Ondemand (Custom)



Rstudio on Ondemand

- We have a guide that show how to use dependencies in Rstudio: https://github.com/kf-cuanschutz/CU-Anschutz-HPC-documentation/tree/main/Rstudio_related_scripts.

Rstudio on Ondemand

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- Use of apptainer, fakeroot and container overlay to modify the container on Alpine.

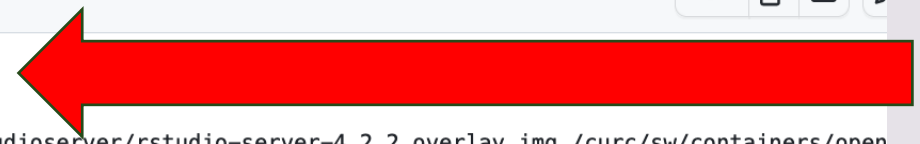
Rstudio on Ondemand

- We have a guide that show how to use dependencies in Rstudio: https://github.com/kf-cuanschutz/CU-Anschutz-HPC-documentation/tree/main/Rstudio_related_scripts.
- Use of apptainer, fakeroot and container overlay to modify the container on Alpine.
- 2 scripts that need to run

Rstudio container

le Blame Executable File · 4 lines (3 loc) · 273 Bytes Raw

```
1  export APPTAINER_TMPDIR=/projects/$USER/.rstudioserver
2  export APPTAINER_CACHEDIR=/projects/$USER/.rstudioserver
3  apptainer shell --fakeroot --overlay /projects/$USER/.rstudioserver/rstudio-server-4.2.2_overlay.img /curc/sw/containers/open
```

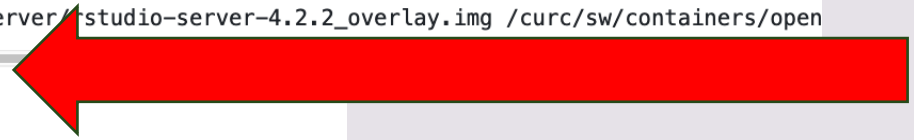


We point the TMPDIR and CACHEDIR to either **/scratch/alpine/$USER** or **/projects/$USER** so that we do not fill /tmp

Rstudio container

le Blame Executable File · 4 lines (3 loc) · 273 Bytes Raw

```
1  export APPTAINER_TMPDIR=/projects/$USER/.rstudioserver
2  export APPTAINER_CACHEDIR=/projects/$USER/.rstudioserver
3  apptainer shell --fakeroot --overlay /projects/$USER/.rstudioserver/rstudio-server-4.2.2_overlay.img /curc/sw/containers/open
```



The overlay with .img
Allows us to modify the .sif container image

Rstudio container

```
apt-get -y update
apt install -y zlib1g-dev
apt install -y libglpk-dev
apt install -y libfftw3-3
apt install -y libcairo2-dev
apt install -y libxt-dev
apt install -y liblzma-dev
apt install -y libharfbuzz-dev
apt install -y libtiff-dev
apt install -y libpng-dev
apt install -y libfribidi-dev
apt install -y libcurl4-openssl-dev
apt install -y libcurl4-nss-dev
apt install -y libcurl4-gnutls-dev
apt install -y libfreetype-dev
apt install -y libbz2-dev
apt install -y libhdf5-dev
```

We install the necessary dependencies inside the container

Run Rstudio container in slurm script

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --time=24:00:00
#SBATCH --qos=normal
#SBATCH --partition=amilan
#SBATCH --ntasks=64
#SBATCH --account=amc-general
#SBATCH --job-name=R_job
#SBATCH --output=Rjob.%j.out
#SBATCH --error=Rjob.%j.err

# Exporting the apptainer tmp directories so that
# we do not fill /tmp
export ALPINE_SCRATCH=/gpfs/alpine1/scratch/$USER
export APPTAINER_TMPDIR=$ALPINE_SCRATCH/singularity/tmp
export APPTAINER_CACHEDIR=$ALPINE_SCRATCH/singularity/cache
mkdir -pv $APPTAINER_CACHEDIR $APPTAINER_TMPD

# Calling the Rstudio container to execute the Rscript
apptainer exec --bind /projects/$USER,/scratch/alpine/$USER --overlay /projects/
$USER/.rstudioserver/rstudio-server-4.2.2_overlay.img:ro /curc/sw/containers/
open_ondemand/rstudio-server-4.2.2.sif Rscript myscript.R
```

The slurm header looks similar to what we have seen before.

Run Rstudio container in slurm script

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --time=24:00:00
#SBATCH --qos=normal
#SBATCH --partition=amilan
#SBATCH --ntasks=64
#SBATCH --account=amc-general
#SBATCH --job-name=R_job
#SBATCH --output=Rjob.%j.out
#SBATCH --error=Rjob.%j.err

# Exporting the apptainer tmp directories so that
# we do not fill /tmp
export ALPINE_SCRATCH=/gpfs/alpine1/scratch/$USER
export APPTAINER_TMPDIR=$ALPINE_SCRATCH/singularity/tmp
export APPTAINER_CACHEDIR=$ALPINE_SCRATCH/singularity/cache
mkdir -pv $APPTAINER_CACHEDIR $APPTAINER_TMPD

# Calling the Rstudio container to execute the Rscript
apptainer exec --bind /projects/$USER,/scratch/alpine/$USER --overlay /projects/
$USER/.rstudioserver/rstudio-server-4.2.2_overlay.img:ro /curc/sw/containers/
open_ondemand/rstudio-server-4.2.2.sif Rscript myscript.R
```

Export tmp related directories to the scratch.

Run Rstudio container in slurm script

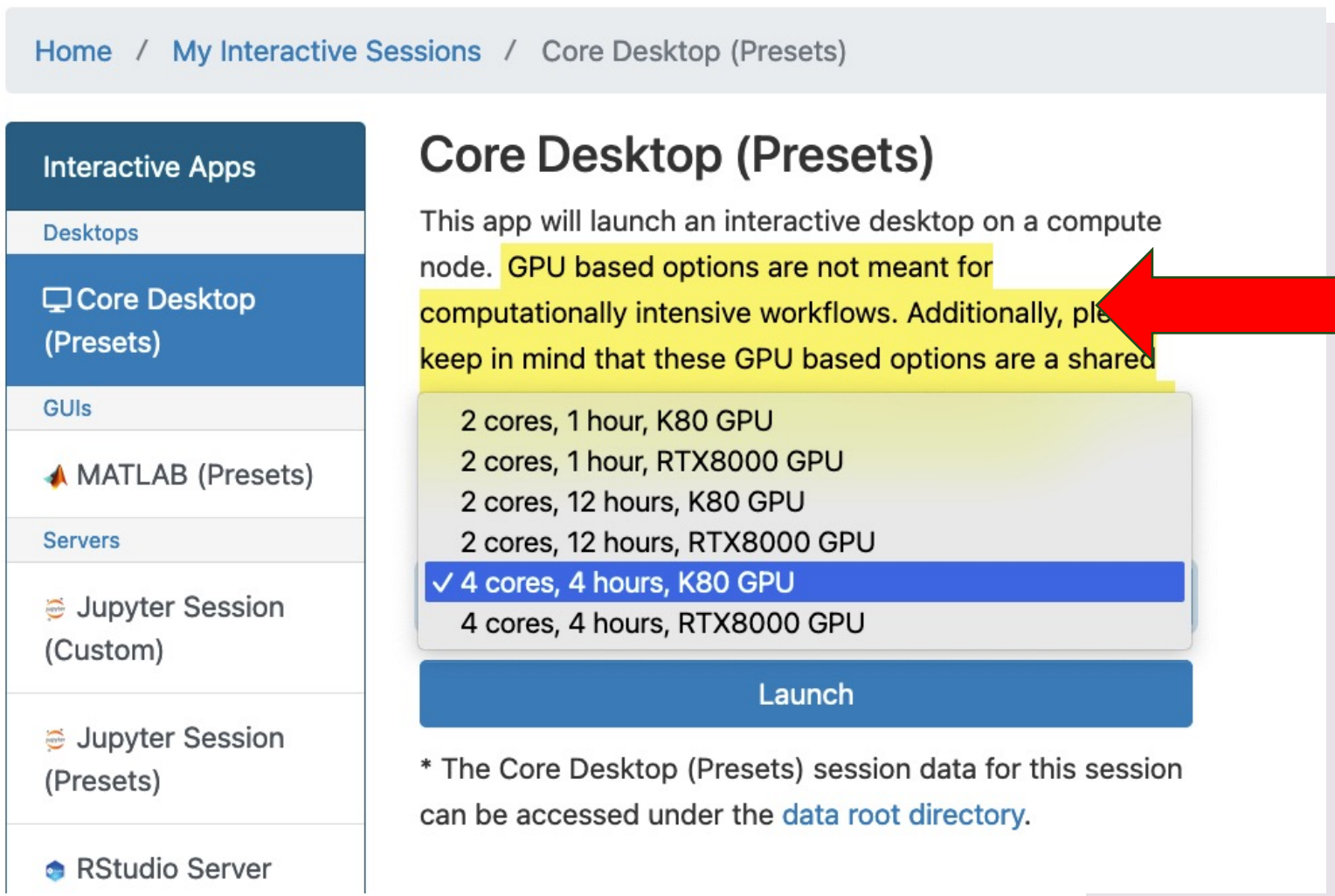
```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --time=24:00:00
#SBATCH --qos=normal
#SBATCH --partition=amilan
#SBATCH --ntasks=64
#SBATCH --account=amc-general
#SBATCH --job-name=R_job
#SBATCH --output=Rjob.%j.out
#SBATCH --error=Rjob.%j.err

# Exporting the apptainer tmp directories so that
# we do not fill /tmp
export ALPINE_SCRATCH=/gpfs/alpine1/scratch/$USER
export APPTAINER_TMPDIR=$ALPINE_SCRATCH/singularity/tmp
export APPTAINER_CACHEDIR=$ALPINE_SCRATCH/singularity/cache
mkdir -pv $APPTAINER_CACHEDIR $APPTAINER_TMPD

# Calling the Rstudio container to execute the Rscript
apptainer exec --bind /projects/$USER,/scratch/alpine/$USER --overlay /projects/
$USER/.rstudioserver/rstudio-server-4.2.2_overlay.img:ro /curc/sw/containers/
open_ondemand/rstudio-server-4.2.2.sif Rscript myscript.R
```

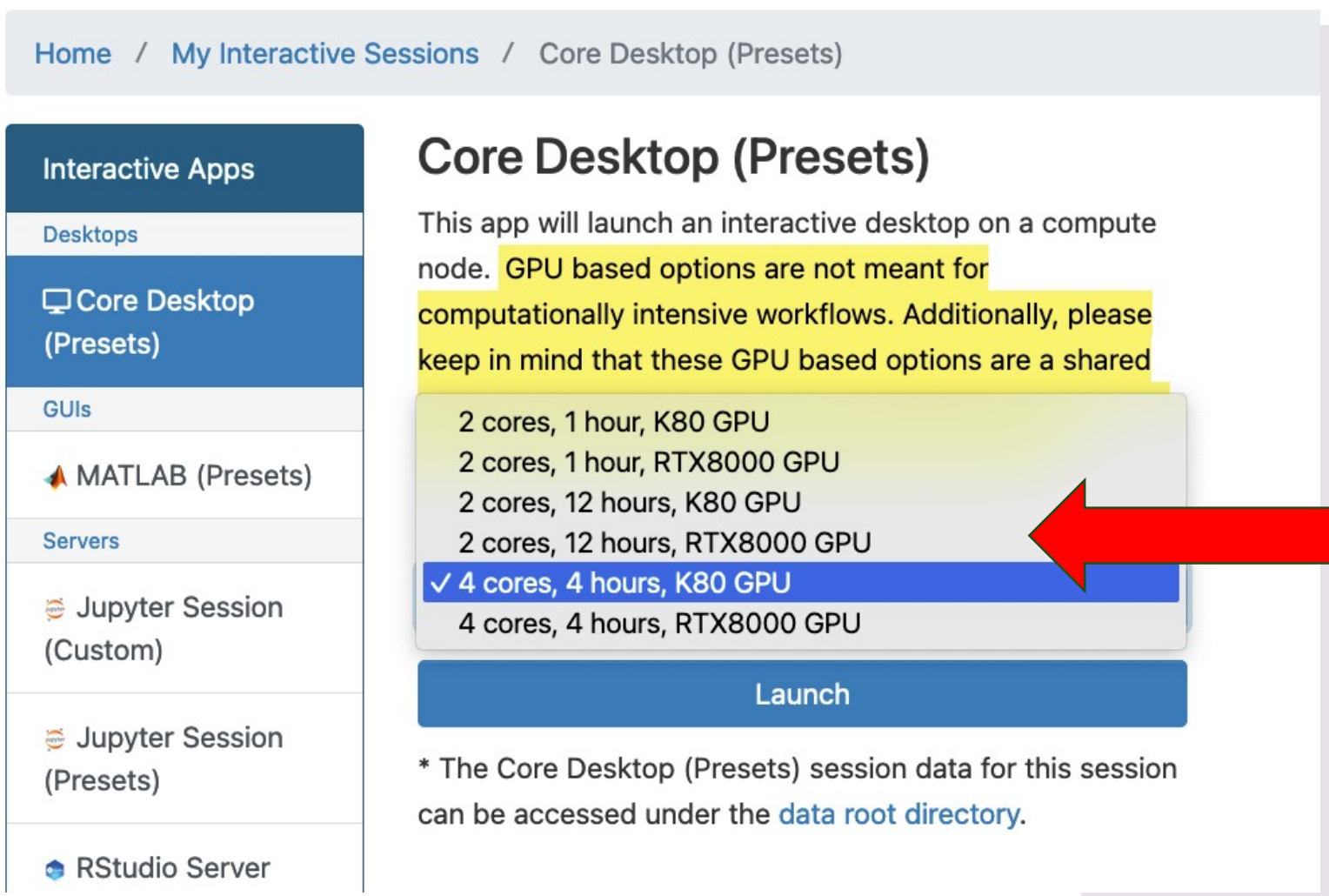
Execute the container with R script.

Core Desktop



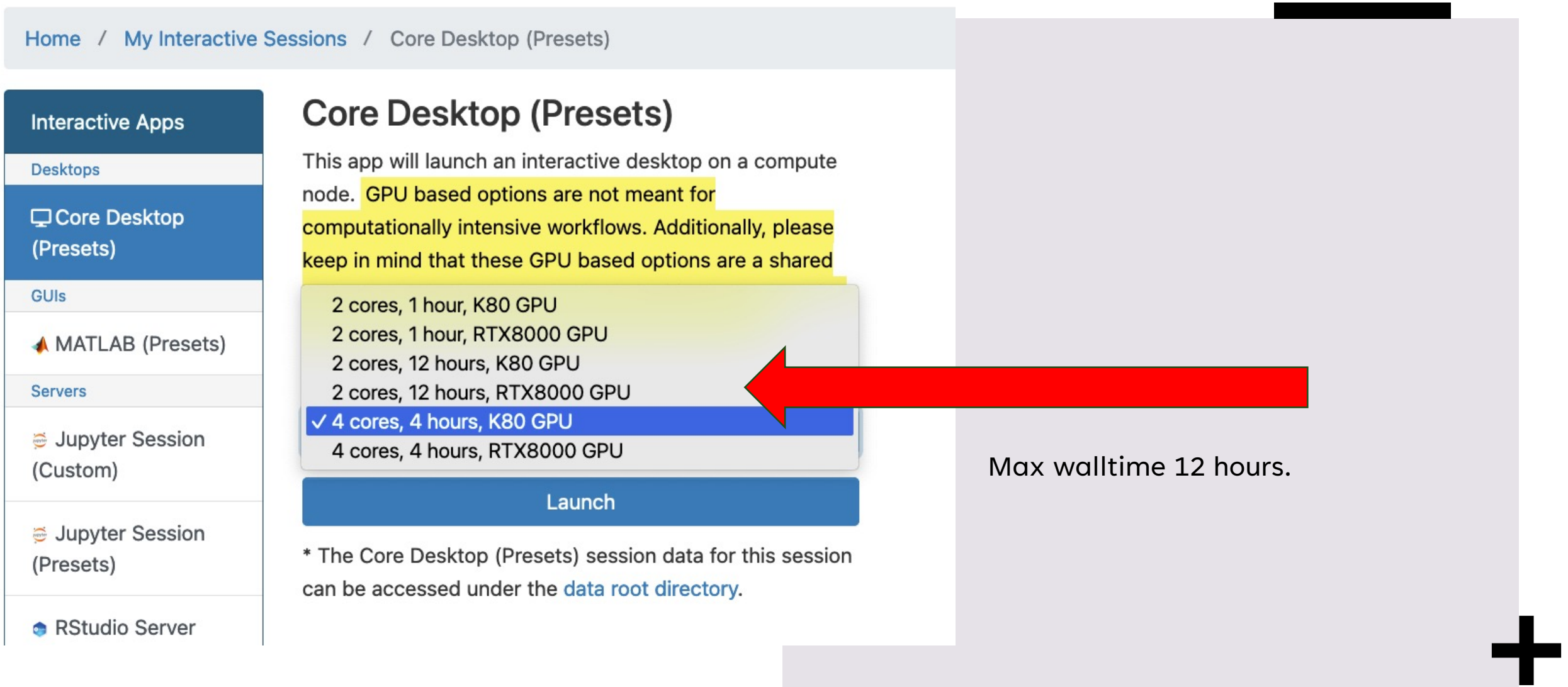
Allows you to interact with a Desktop like env

Core Desktop



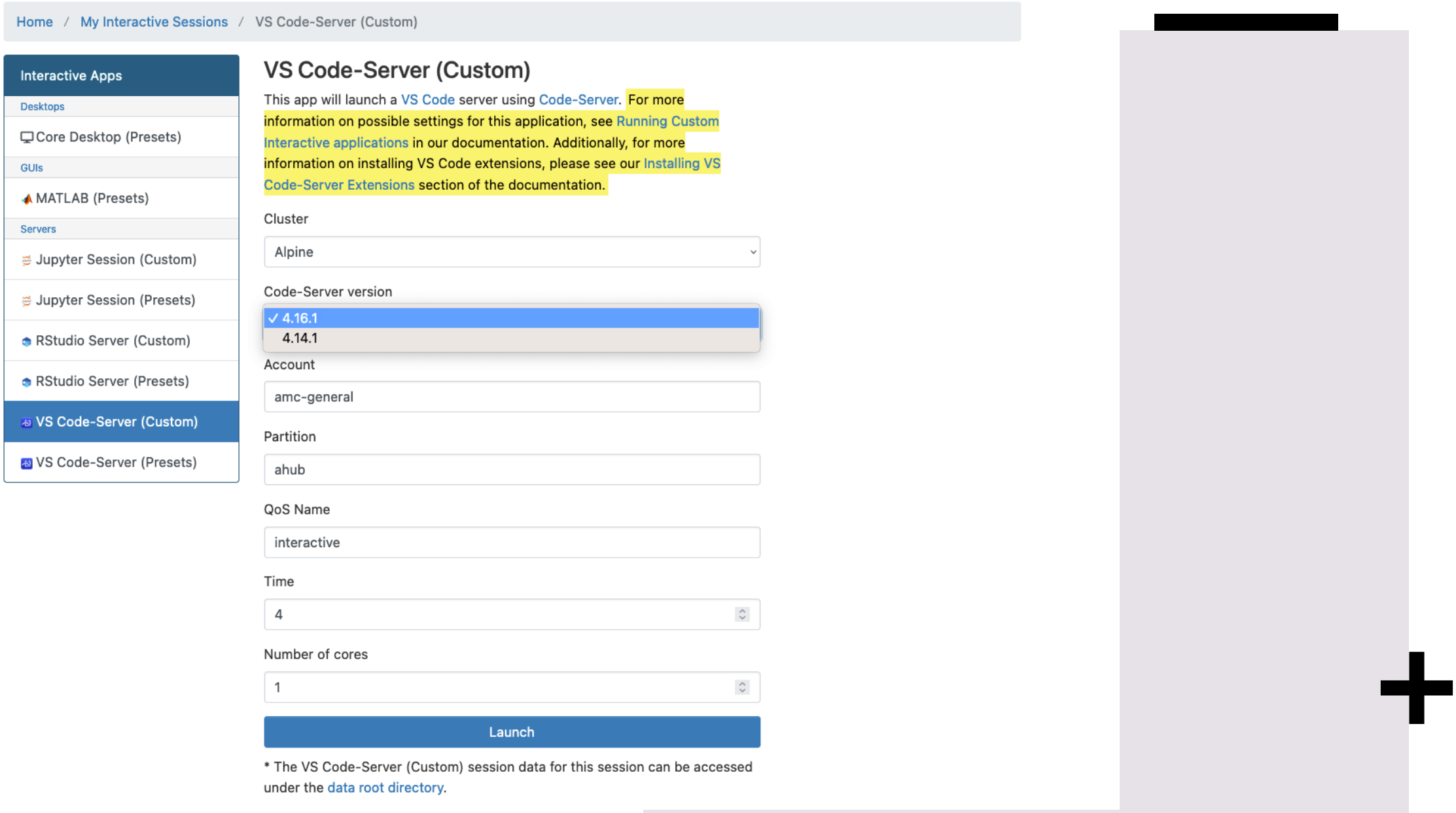
2 types of GPUs: RTX8000 and K80

Core Desktop

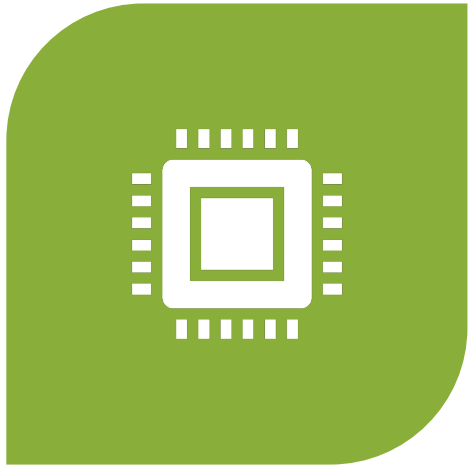


Max walltime 12 hours.

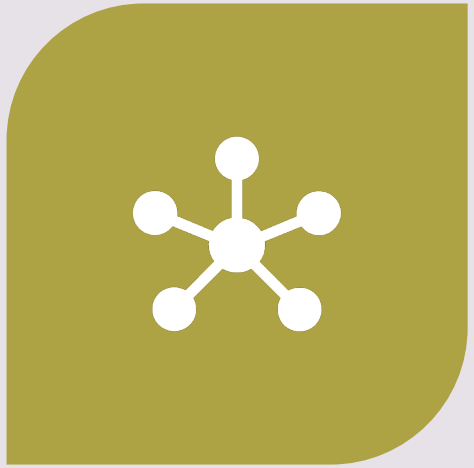
VS Code on Ondemand-rmacc



GPU nodes on Alpine



12 NVIDIA GPU NODES (3 GPU EACH)



8 AMD GPU NODES (3 GPU EACH)

GPU partition on Alpine

aa100 -> NVIDIA RELATED PARTITION; MAX WALLTIME 24 HOURS

ami100 -> AMD RELATED PARTITION; MAX WALLTIME 24 HOURS

atesting_a100 -> NVIDIA TESTING PARTITION; MAX WALLTIME 1 HOUR

atesting_mi100 -> AMD TESTING PARTITION; MAX WALLTIME 1 HOUR

Important: to request more than 24 hours walltime use:

--qos=long

Access to NVIDIA Job partition

```
#!/bin/bash

#SBATCH --job-name=full_genome_nn_hp_opt_gpu
#SBATCH --output=full_genome_nn_hp_opt_gpu.out
#SBATCH --error=full_genome_nn_hp_opt_gpu.err
#SBATCH --partition=aa100
#SBATCH --nodes=1
#SBATCH --ntasks=45
#SBATCH --gres=gpu:1
#SBATCH --account=amc-general
#SBATCH --time=24:00:00
```

- To access an AMD partition add: **--partition=ami100**
- Here, the number of gpus are allocated with: **--gres=gpu:1**

Debug nodes for NVIDIA A100 and AMD MI100

[NVIDIA] sinteractive

--partition=atesting_a100 --qos=testing

--time=00:05:00 --gres=gpu:1 --ntasks=2

[AMD] sinteractive

--partition=atesting_mi100 --qos=testing

--time=00:05:00 --gres=gpu:1 --ntasks=2

Users are now limited to up to 2/3 of the GPU partition (not per node)

Package availability for ML (2)

- Cuda versions 11.2, 11.3, 11.4, 11.8 and 12.1.1 on Alpine.
- Only cudnn 8.1, 8.2 and 8.6 on Alpine.

GPU

Version	Python version	Compiler	Build tools	cuDNN	CUDA
tensorflow-2.13.0	3.8-3.11	Clang 16.0.0	Bazel 5.3.0	8.6	11.8
tensorflow-2.12.0	3.8-3.11	GCC 9.3.1	Bazel 5.3.0	8.6	11.8
tensorflow-2.11.0	3.7-3.10	GCC 9.3.1	Bazel 5.3.0	8.1	11.2
tensorflow-2.10.0	3.7-3.10	GCC 9.3.1	Bazel 5.1.1	8.1	11.2
tensorflow-2.9.0	3.7-3.10	GCC 9.3.1	Bazel 5.0.0	8.1	11.2
tensorflow-2.8.0	3.7-3.10	GCC 7.3.1	Bazel 4.2.1	8.1	11.2
tensorflow-2.7.0	3.7-3.9	GCC 7.3.1	Bazel 3.7.2	8.1	11.2
tensorflow-2.6.0	3.6-3.9	GCC 7.3.1	Bazel 3.7.2	8.1	11.2
tensorflow-2.5.0	3.6-3.9	GCC 7.3.1	Bazel 3.7.2	8.1	11.2
tensorflow-2.4.0	3.6-3.8	GCC 7.3.1	Bazel 3.1.0	8.0	11.0
tensorflow-2.3.0	3.5-3.8	GCC 7.3.1	Bazel 3.1.0	7.6	10.1

Pytorch installation on Alpine [NVIDIA] (1)

1. After you log into the Alpine cluster, please load the slurm modules and request allocation so that you can install the packages:

```
module load slurm/alpine
acompile --ntasks=4
```

2. Load anaconda, create your environment with python 3.10 and activate it.

```
module load anaconda
conda create -n pytorch_env python=3.10
conda activate pytorch_env
```

3. Install pytorch, pytorch-cuda. You could also install torchvision and torchaudio if needed for your workflow.

```
conda install pytorch==2.0.0 torchvision==0.15.0 torchaudio==2.0.0 pytorch-cuda=11.8 -c pytorch -c nvidia
```

4. Install cuda-toolkit 11.8.0

```
conda install -c "nvidia/label/cuda-11.8.0" cuda-toolkit
```

Pytorch installation on Alpine [NVIDIA] (2)

5. Install nvidia-cudnn 8.6.0

```
pip install nvidia-cudnn-cu11==8.6.0.163
```

6. To test that your installation is working you will need to exit "acompile" first and load on the NVIDIA gpu debug partition on Alpine"

```
conda deactivate
exit
sinteractive --partition=atesting_a100 --qos=testing --time=00:05:00 --gres=gpu:1 --ntasks=2
module load anaconda
conda activate pytorch_env
python
```

7. Finally, run the following:

```
>>>import torch
>>>print(torch.cuda.is_available())
True
```

8. Make sure to exit the GPU debug node partition after testing the installation.

```
$ exit
exit
```

Tensorflow installation on Alpine [NVIDIA] (1)

1. After you log into the Alpine cluster, please load the Slurm modules and request allocation so that you can install the packages:

```
module load slurm/alpine
acompile --ntasks=4 --time=01:30:00
```

2. Load anaconda, create your environment with python 3.9 and activate it.

```
module load anaconda
conda create -n tf_env python=3.9
conda activate tf_env
```

3. Install cudnn 8.6.0

```
pip install nvidia-cudnn-cu11==8.6.0.163
```

4. Install cuda-toolkit 11.8.0

```
conda install -c "nvidia/label/cuda-11.8.0" cuda-toolkit
```

Tensorflow installation on Alpine [NVIDIA] (2)

5. Install Tensorflow 2.12.0. Also note that tensorflow, cuda and cudnn have to follow a strict versioning: https://www.tensorflow.org/install/source#gpu

```
python3 -m pip install tensorflow==2.12.0
```

6. Export the correct paths by following this guide here: https://www.tensorflow.org/install/pip

```
mkdir -p $CONDA_PREFIX/etc/conda/activate.d
echo 'CUDNN_PATH=$(dirname $(python -c "import nvidia.cudnn;print(nvidia.cudnn.__file__)"))' >> $CONDA_PREFIX/etc/co
echo 'export LD_LIBRARY_PATH=$CONDA_PREFIX/lib/:$CUDNN_PATH/lib:$LD_LIBRARY_PATH' >> $CONDA_PREFIX/etc/conda/activat
source $CONDA_PREFIX/etc/conda/activate.d/env_vars.sh
export LD_LIBRARY_PATH=$CONDA_PREFIX/lib/python3.9/site-packages/nvidia/cudnn/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=$CONDA_PREFIX/lib:$LD_LIBRARY_PATH
export PATH=$CONDA_PREFIX/bin:$PATH
export XLA_FLAGS=--xla_gpu_cuda_data_dir=$CONDA_PREFIX
```

7. Install Tensorrt and export PATH:

```
pip install nvidia-tensorrt==8.4.1.5
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$CONDA_PREFIX/lib/python3.9/site-packages/tensorrt
```

Tensorflow installation on Alpine [NVIDIA] (3)

8. We link libnvinfer.so.8 to libnvinfer.so.7 :

```
ln -s $CONDA_PREFIX/lib/python3.9/site-packages/tensorrt/libnvinfer.so.8 $CONDA_PREFIX/lib/python3.9/site-packages/t
ln -s $CONDA_PREFIX/lib/python3.9/site-packages/tensorrt/libnvinfer_plugin.so.8  $CONDA_PREFIX/lib/python3.9/site-pa
```

9. To test that your installation is working you will need to exit "acompile" first and load on the NVIDIA GPU debug partition on Alpine"

```
conda deactivate
exit
sinteractive --partition=atesting_a100 --qos=testing --time=00:05:00 --gres=gpu:1 --ntasks=2
module load anaconda
conda activate tf_env
python3 -c "import tensorflow as tf; print(tf.config.list_physical_devices('GPU'))"
```

10. Make sure to exit the GPU debug node partition after testing the installation.

```
$ exit
exit
```

Slurm script for AMD GPU partition

```
#!/bin/bash
#SBATCH --job-name=run_amd_gpu_standard
#SBATCH --output=run_amd_gpu_standard.%j.out
#SBATCH --error=run_amd_gpu_standard.%j.err
#SBATCH --partition=ami100
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=6
#SBATCH --gres=gpu:1
#SBATCH --account=amc-general
#SBATCH --reservation=amc_workshop
#SBATCH --time=00:10:00


# We make sure that the user can run mambaforge
cp ~/.condarc ~/.mambarc

echo "********************************** Loading ROCM and pytorch + exporting useful paths  **********************************"
# We load ROCM which is the collection of drivers, libraries, tools and API to run
# on an AMD GPU : https://rocm.docs.amd.com/en/latest/what-is-rocm.html
# For NVIDIA it is NVIDIA CUDA
module load rocm/5.2.3

# We load pytorch 1.13.0 that has been built for the ROCM,
# which is compatible with ROCM5.2.X : https://pytorch.org/get-started/previous-versions/
module load pytorch/1.13.0
```

We give job name, output and error

Slurm script for AMD GPU partition

```
#!/bin/bash
#SBATCH --job-name=run_amd_gpu_standard
#SBATCH --output=run_amd_gpu_standard.%j.out
#SBATCH --error=run_amd_gpu_standard.%j.err
#SBATCH --partition=ami100
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=6
#SBATCH --gres=gpu:1
#SBATCH --account=amc-general
#SBATCH --reservation=amc_workshop
#SBATCH --time=00:10:00


# We make sure that the user can run mambaforge
cp ~/.condarc ~/.mambarc

echo "********************************** Loading ROCM and pytorch + exporting useful paths  **********************************"
# We load ROCM which is the collection of drivers, libraries, tools and API to run
# on an AMD GPU : https://rocm.docs.amd.com/en/latest/what-is-rocm.html
# For NVIDIA it is NVIDIA CUDA
module load rocm/5.2.3

# We load pytorch 1.13.0 that has been built for the ROCM,
# which is compatible with ROCM5.2.X : https://pytorch.org/get-started/previous-versions/
module load pytorch/1.13.0
```

Name of the AMD GPU partition

Slurm script for AMD GPU partition

```
#!/bin/bash
#SBATCH --job-name=run_amd_gpu_standard
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module load pytorch/1.13.0
```

We ask for 1 node and a few cores since most computati on will be on the gpu

Slurm script for AMD GPU partition

```
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#SBATCH --error=run_amd_gpu_standard.%j.err
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# which is compatible with ROCM5.2.X : https://pytorch.org/get-started/previous-versions/
module load pytorch/1.13.0
```

We ask for
1 GPU

Slurm script for AMD GPU partition

```
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#SBATCH --job-name=run_amd_gpu_standard
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#SBATCH --error=run_amd_gpu_standard.%j.err
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# which is compatible with ROCM5.2.X : https://pytorch.org/get-started/previous-versions/
module load pytorch/1.13.0
```

We load the modules

Slurm script for AMD GPU partition

```
echo "********************************** Running the models  **********************************"
# We want to make sure that we can profile what is going on
# We want to set AMD_LOG_LEVEL for profiling and debugging
#CODE 0 means No log
#CODE 1 means log the error
#CODE 2 means log warnings
#CODE 3 means log information
#CODE 4 means debug mode
# More information here: https://rocm.docs.amd.com/projects/HIP/en/develop/developer_guide/logging.html

HIP_VISIBLE_DEVICES=0 ROCR_VISIBLE_DEVICES=0 AMD_LOG_LEVEL=1 HSA_ENABLE_SDMA=0 python tensors.py
```

Here is a way we can debug our code or even profile what is going on

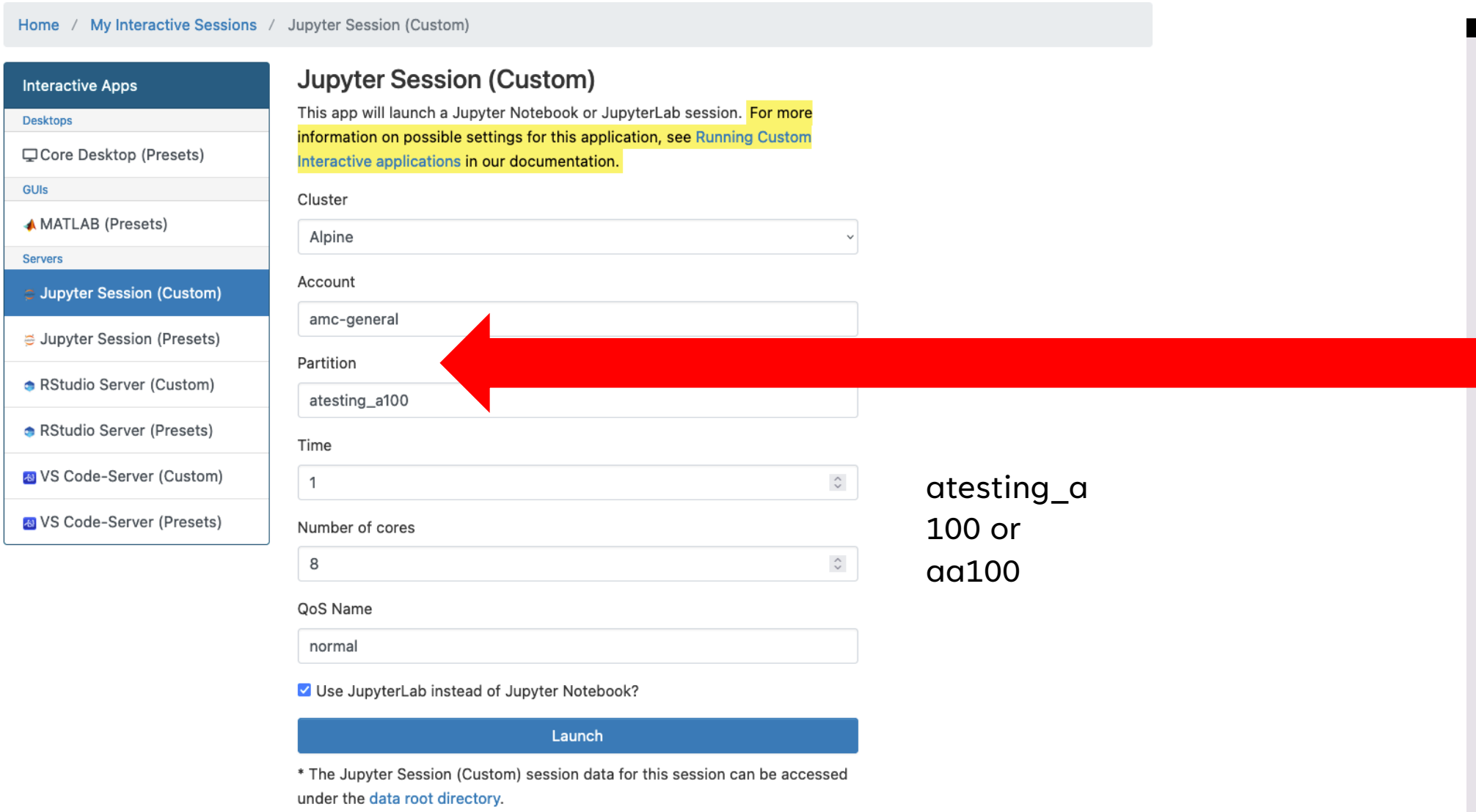
Slurm script for AMD GPU partition

```
echo "********************************** Running the models  **********************************"
# We want to make sure that we can profile what is going on
# We want to set AMD_LOG_LEVEL for profiling and debugging
#CODE 0 means No log
#CODE 1 means log the error
#CODE 2 means log warnings
#CODE 3 means log information
#CODE 4 means debug mode
# More information here: https://rocm.docs.amd.com/projects/HIP/en/develop/developer_guide/logging.html

HIP_VISIBLE_DEVICES=0 ROCR_VISIBLE_DEVICES=0 AMD_LOG_LEVEL=1 HSA_ENABLE_SDMA=0 python tensors.py
```

AMD_LOG_LEVEL variable is very useful

Jupyterhub with NVIDIA GPUs on Ondemand



atesting_a
100 or
aa100

Containers (1)

- Apptainer/Singularity can now be built directly on the cluster
- Can be built either from a definition file or converted from a docker image.
- e.g: `apptainer build -f R_spack_env.sif R_spack_env.def`

Containers (2)

- acompile --ntasks=4 –time=04:00:00
  - export ALPINE_SCRATCH=/gpfs/alpine1/scratch/$USER
  - export APPTAINER_TMPDIR=$ALPINE_SCRATCH/singularity/tmp
  - export APPTAINER_CACHEDIR=$ALPINE_SCRATCH/singularity/cache
  - mkdir -pv $APPTAINER_CACHEDIR $APPTAINER_TMPD

Exporting the TMP related directories

Containers (2)

- acompile --ntasks=4 –time=04:00:00
  - export ALPINE_SCRATCH=/gpfs/alpine1/scratch/$USER
  - export APPTAINER_TMPDIR=$ALPINE_SCRATCH/singularity/tmp
  - export APPTAINER_CACHEDIR=$ALPINE_SCRATCH/singularity/cache
  - mkdir -pv $APPTAINER_CACHEDIR $APPTAINER_TMPD
- apptainer build deepvariant.sif **docker://**google/deepvariant:"${BIN_VERSION}"

Always add docker:// when building from a docker container

Questions?

Let’s a go!!