University of Colorado **Anschutz Medical Campus**

Overview of Alpine

By AMC HPC and Research Computing
11/25/2024

I- Attending Team Members

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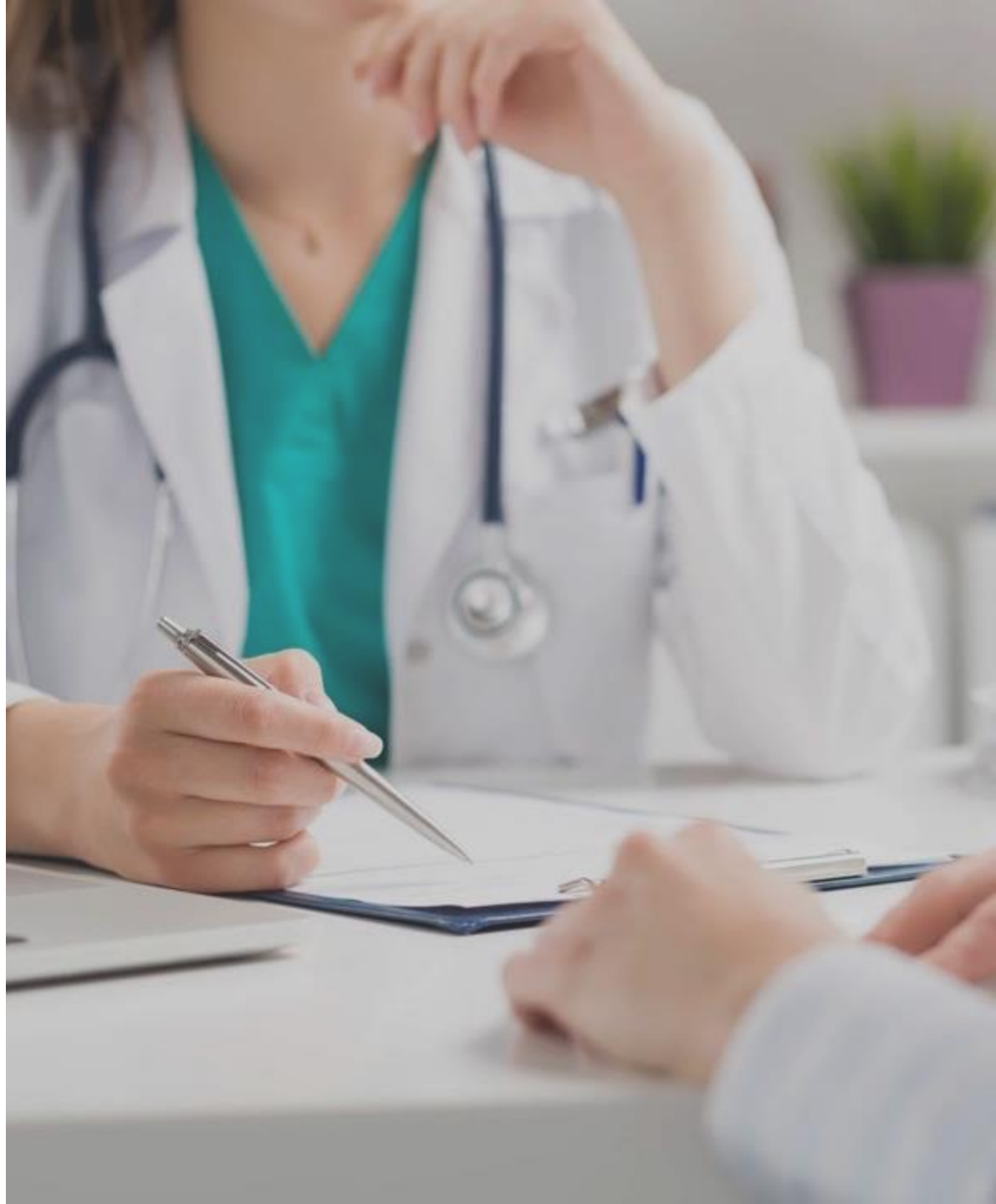
Attending Team Members

- Kevin Fotso: Bioinformatics Technical Analyst.
- Maclean Sherren: Bioinformatics Technical Analyst.



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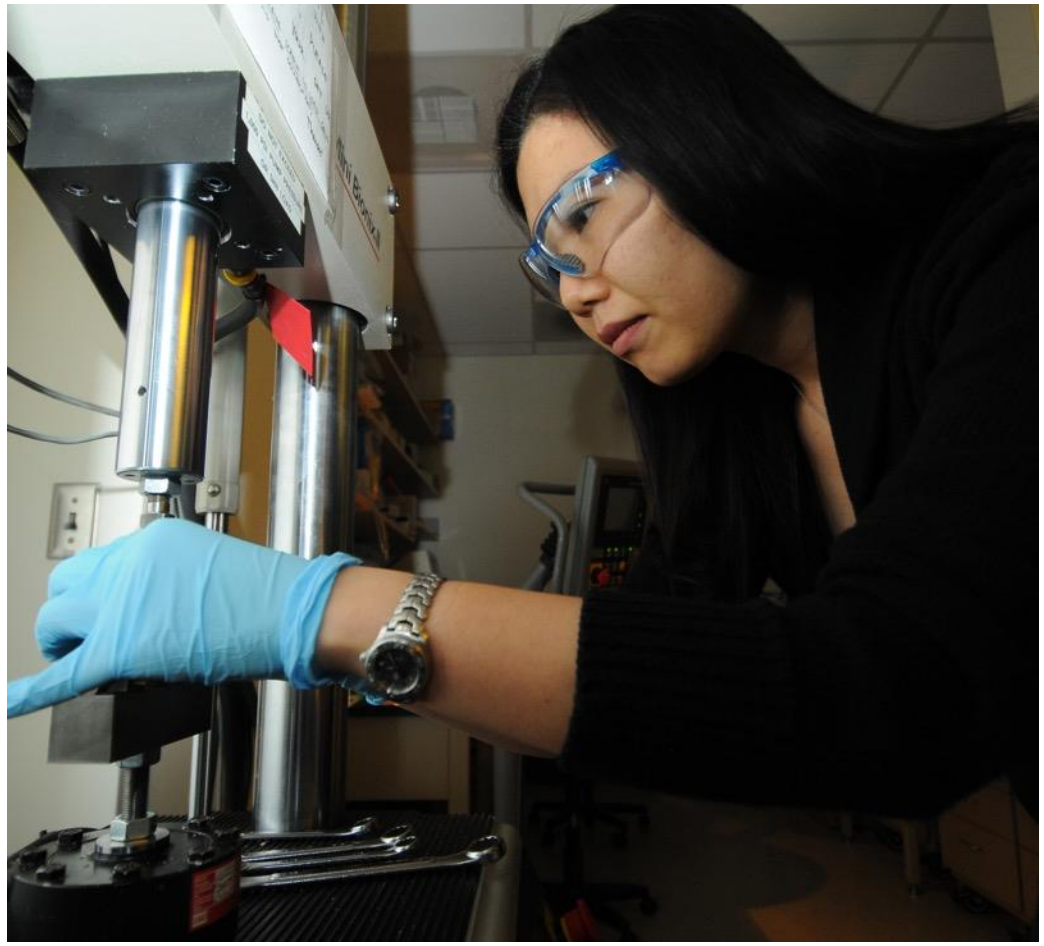
II- What is Alpine?

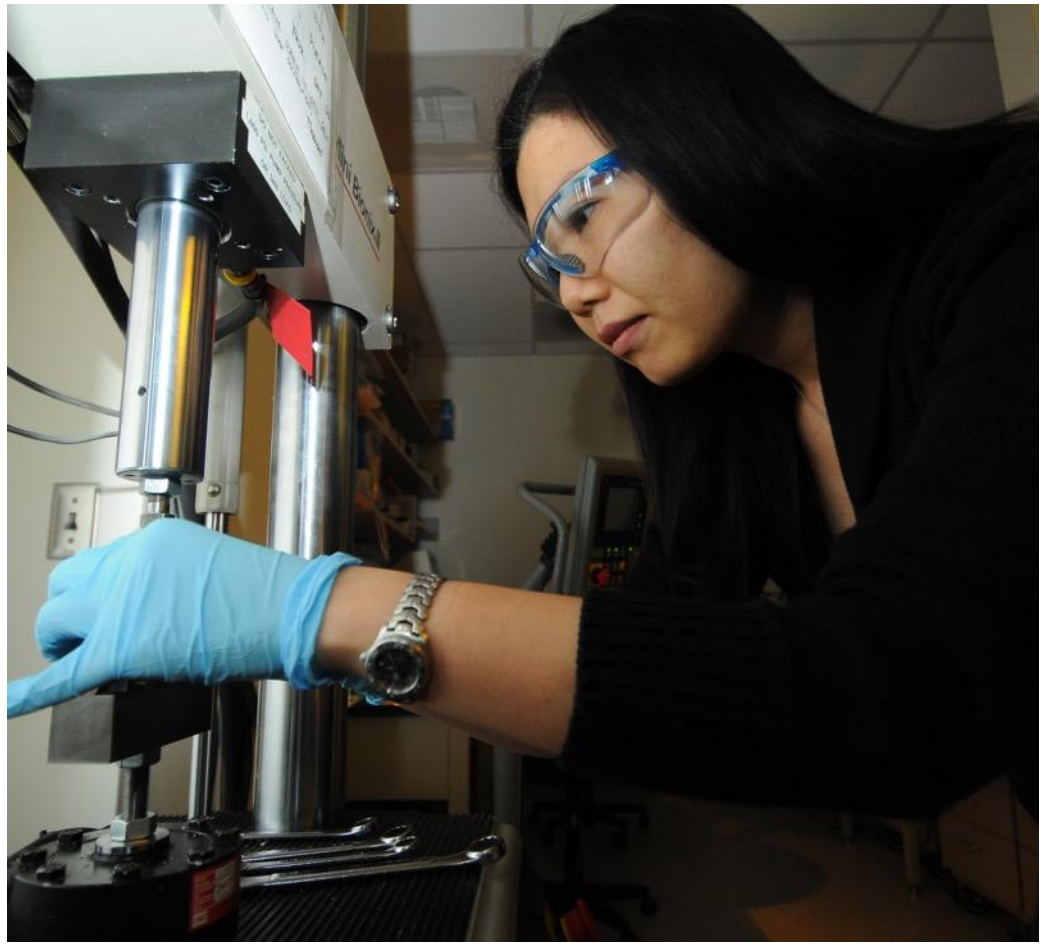
What is Alpine?

Alpine is a supercomputing cluster funded by institutional contributions from the University of Colorado Boulder (UCB), the University of Colorado Anschutz Medical Campus (AMC), Colorado State University (CSU), and by National Science Foundation grants.



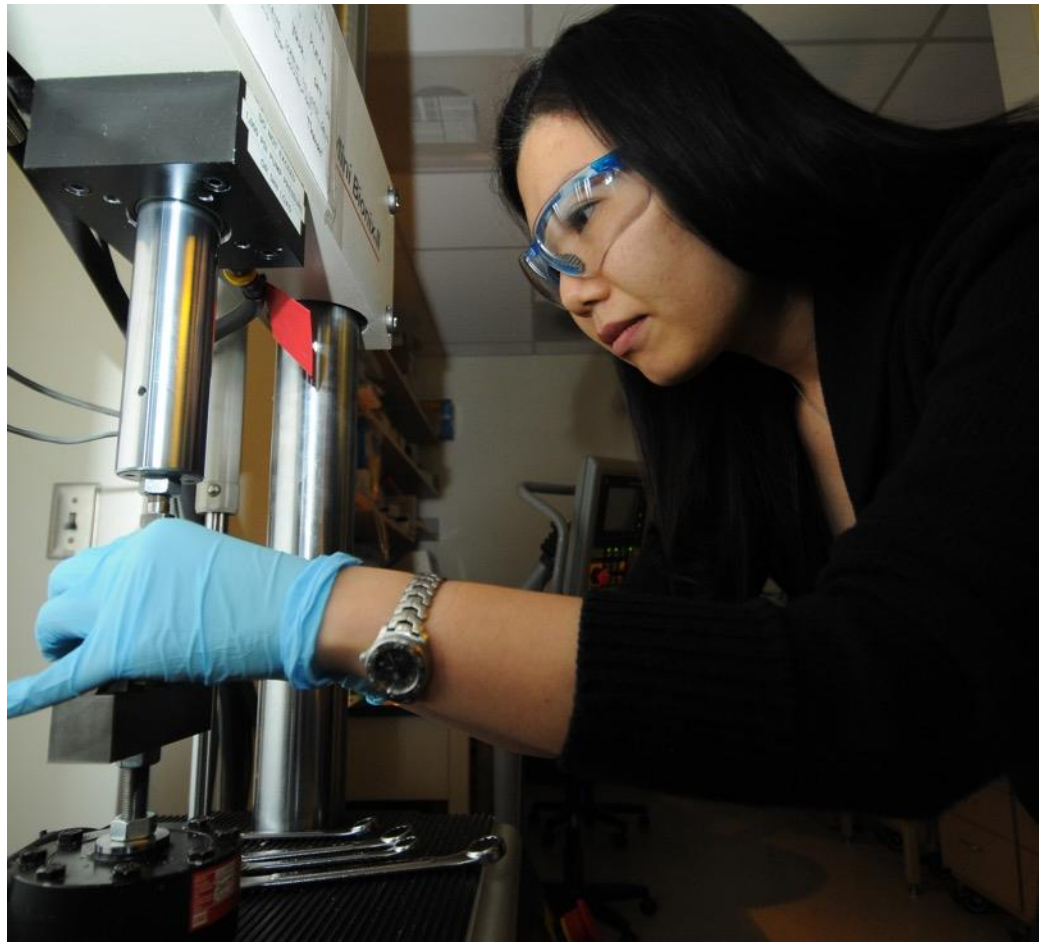
What is Alpine?

It is available to any US-based researcher affiliated with UCB, AMC, CSU, and institutions that are members of the Rocky Mountain Advanced Computing Consortium (RMACC).



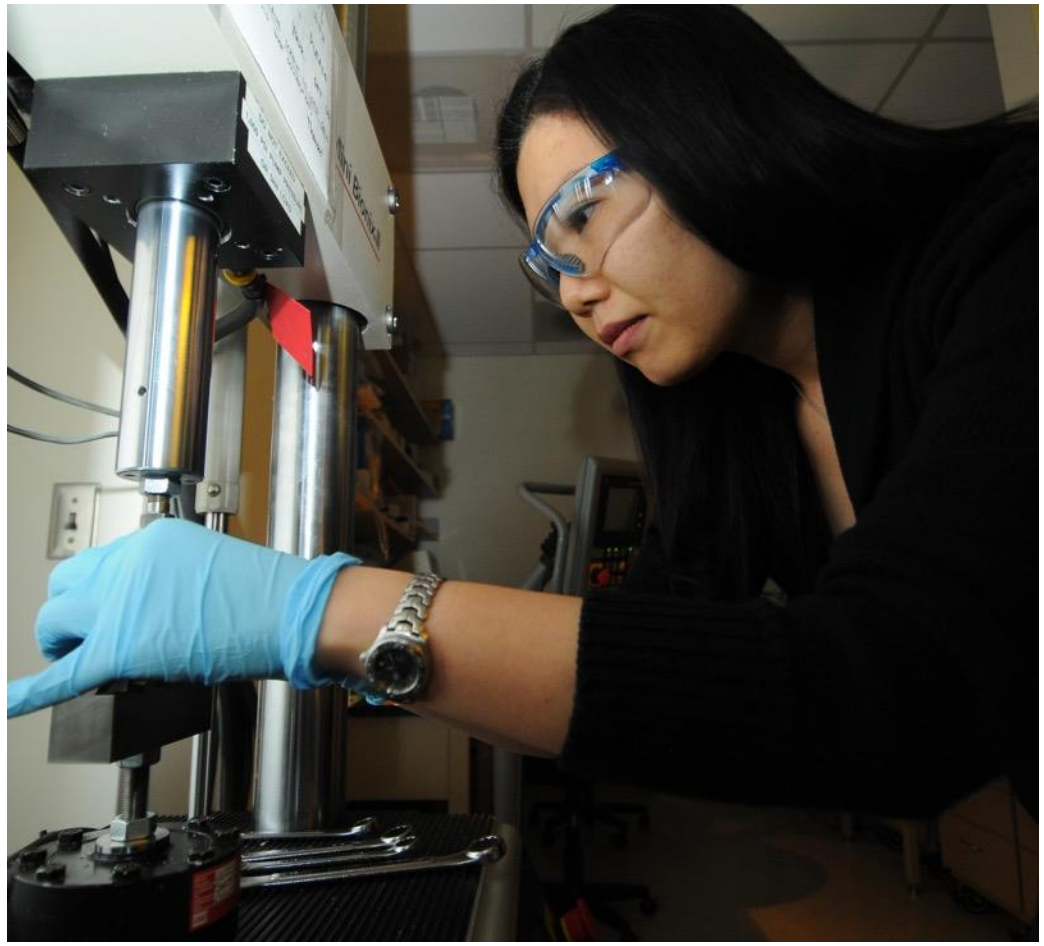
What is Alpine?

- Alpine uses slurm as the scheduler to allocate resources for jobs.



What is Alpine?

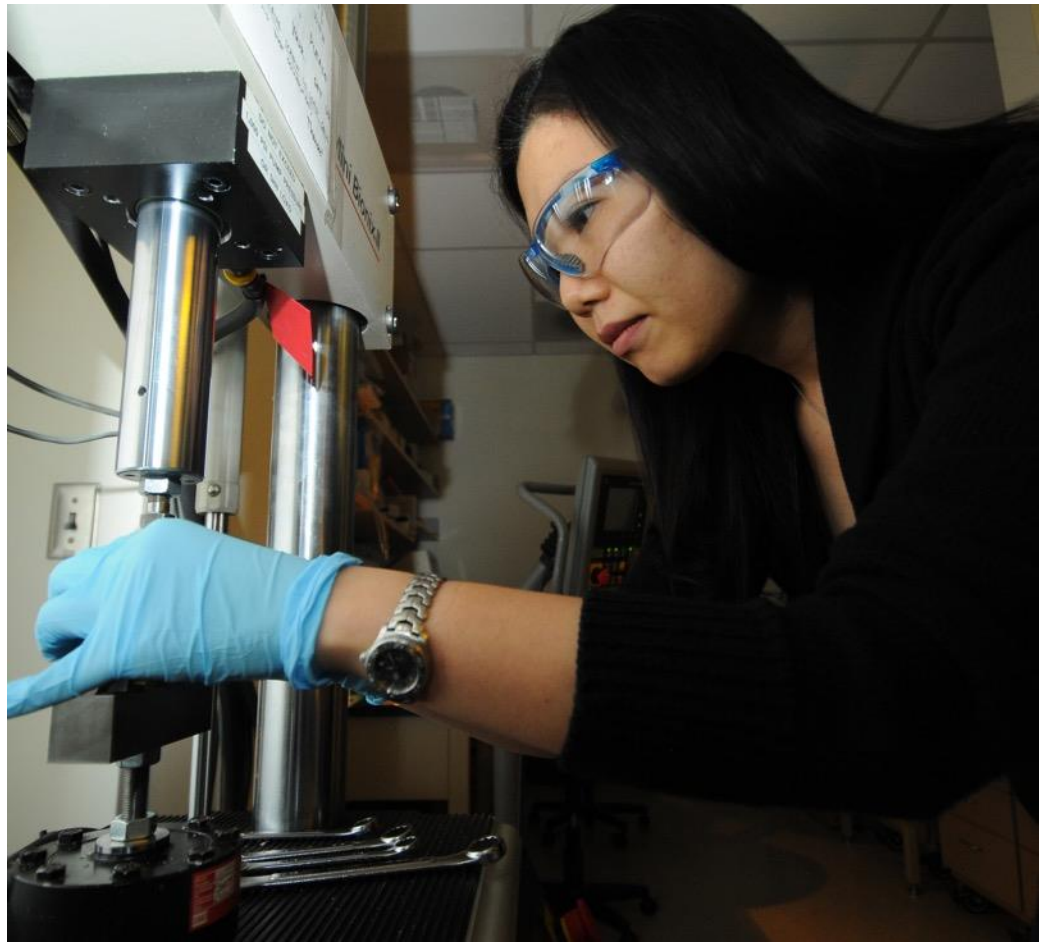
- Alpine uses slurm as the scheduler to allocate resources for jobs.
- Slurm is an open source, fault-tolerant, and highly scalable cluster management and job scheduling system for large and small Linux clusters.



Source: https://slurm.schedmd.com/quickstart.html

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.
- No highly confidential data.
- More information here: https://www.colorado.edu/rc/resources/petalibrary/tos



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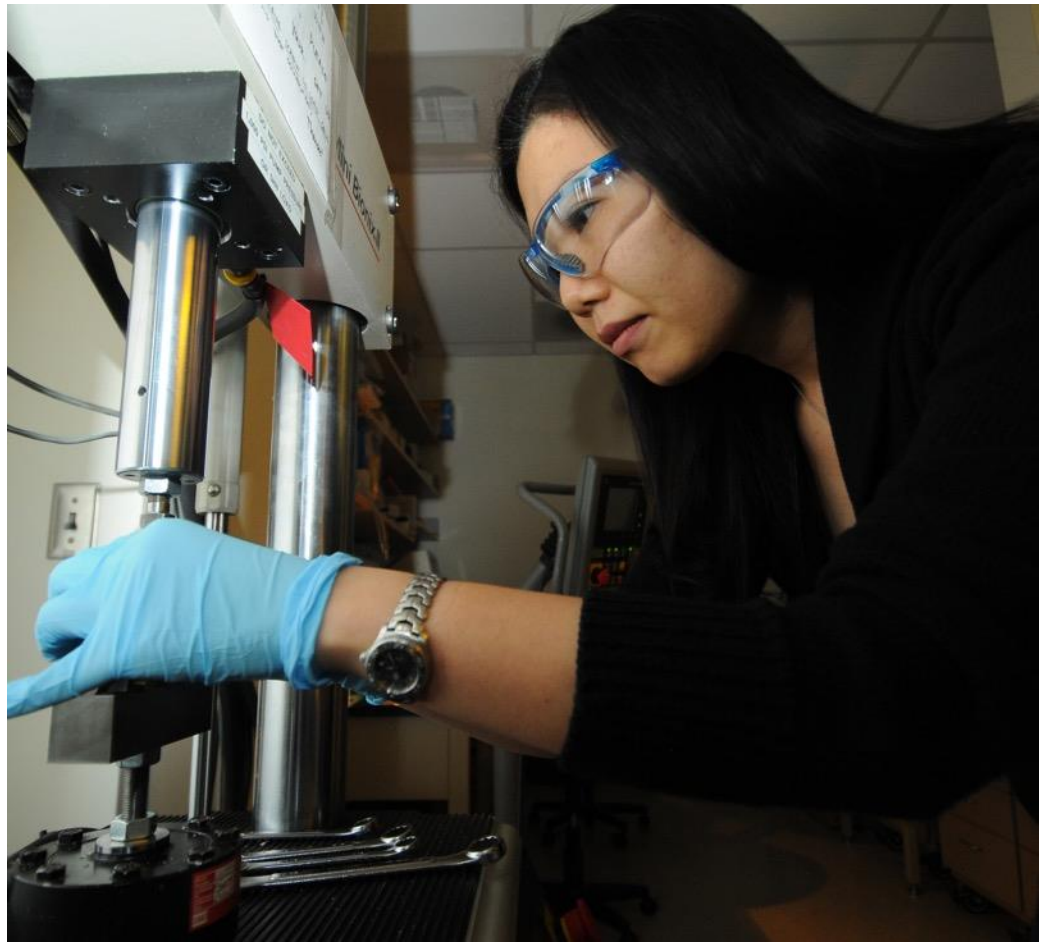
- More information here: https://www.colorado.edu/rc/resources/petalibrary/tos
- Data classification: https://www.cu.edu/security/data-classification.
- HIPAA identifiers: https://www.dhcs.ca.gov/dataandstats/data/Pages/ListofHIPAAIdentifiers.aspx
- Alpine EUA form: https://ucdenverdata.formstack.com/forms/alpine_eua_and_intake



Alpine EUA form

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Anschutz Medical Campus Research Computing End User Agreement

Introduction

This End User Agreement (EUA) is made by and between the Anschutz Medical Campus (CU Anschutz) High Performance Computing (HPC) system user and the Regents of the University of Colorado, a body corporate, for and on behalf of the University of Colorado Denver | Anschutz Medical Campus Office of Information Technology (OIT) concerning the use of University of Colorado Research Computing (CURC) systems housed at the University of Colorado | Boulder.

These systems include but are not limited to the use of Summit, Alpine, Blanca, CUmulus, and the PetaLibrary. These systems are not designed to support computing on data covered by regulatory requirements such HIPAA, GDPR (e.g. UK Biobank), or FERPA data. This page highlights potential HIPAA identifiers. Finally, any credentials associated with PHI accounts such as the Health Data Compass Google credentials cannot be used on Alpine nor can the credentials and their corresponding keys and/or tokens be stored on Alpine. For more information about the Alpine HPC system and other services offered by CURC, please click here.

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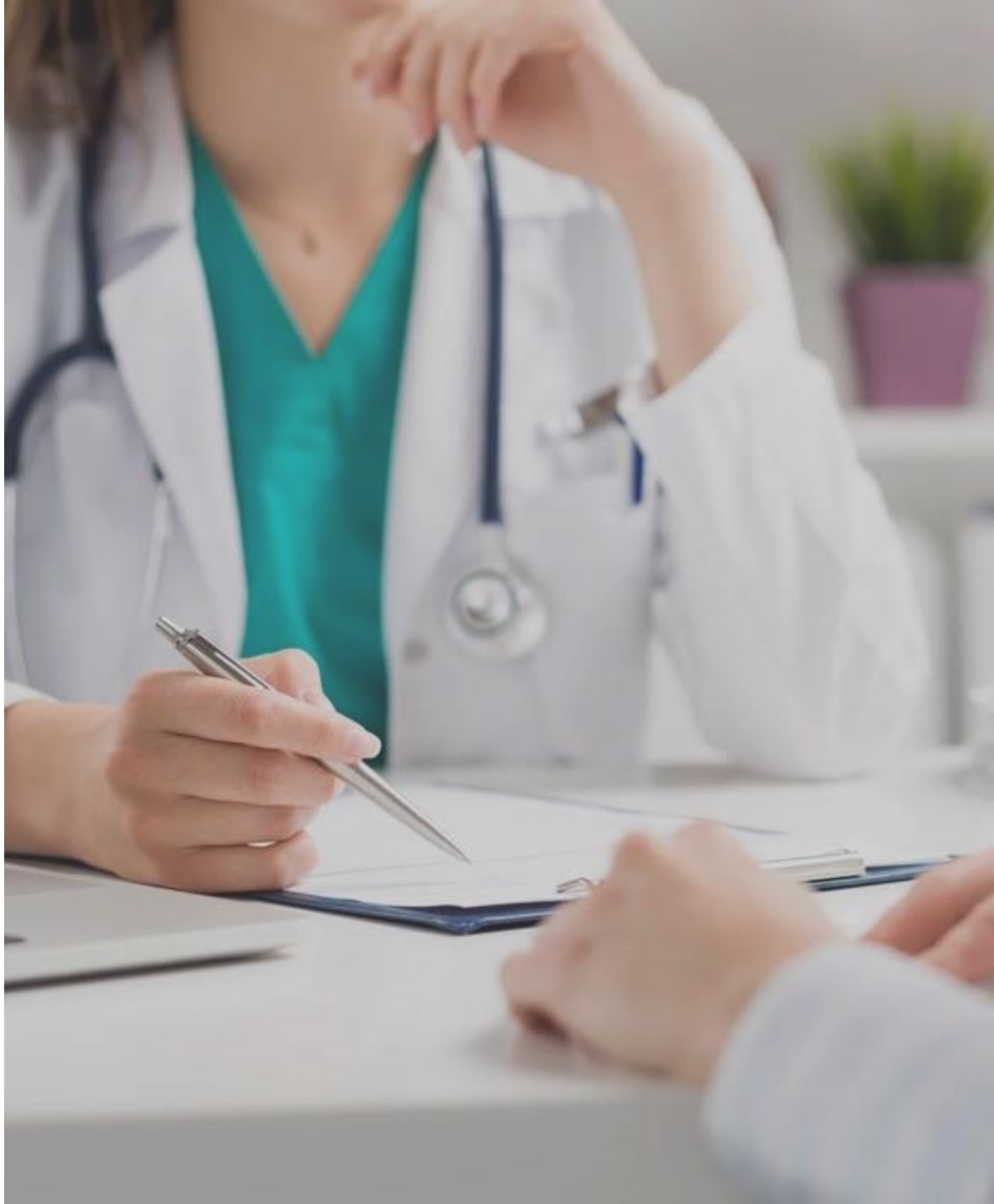
Source: *https://ucdenverdata.formstack.com/forms/alpine_eua_and_intake*

III- Alpine nodes

Alpine nodes

- 389 nodes in total



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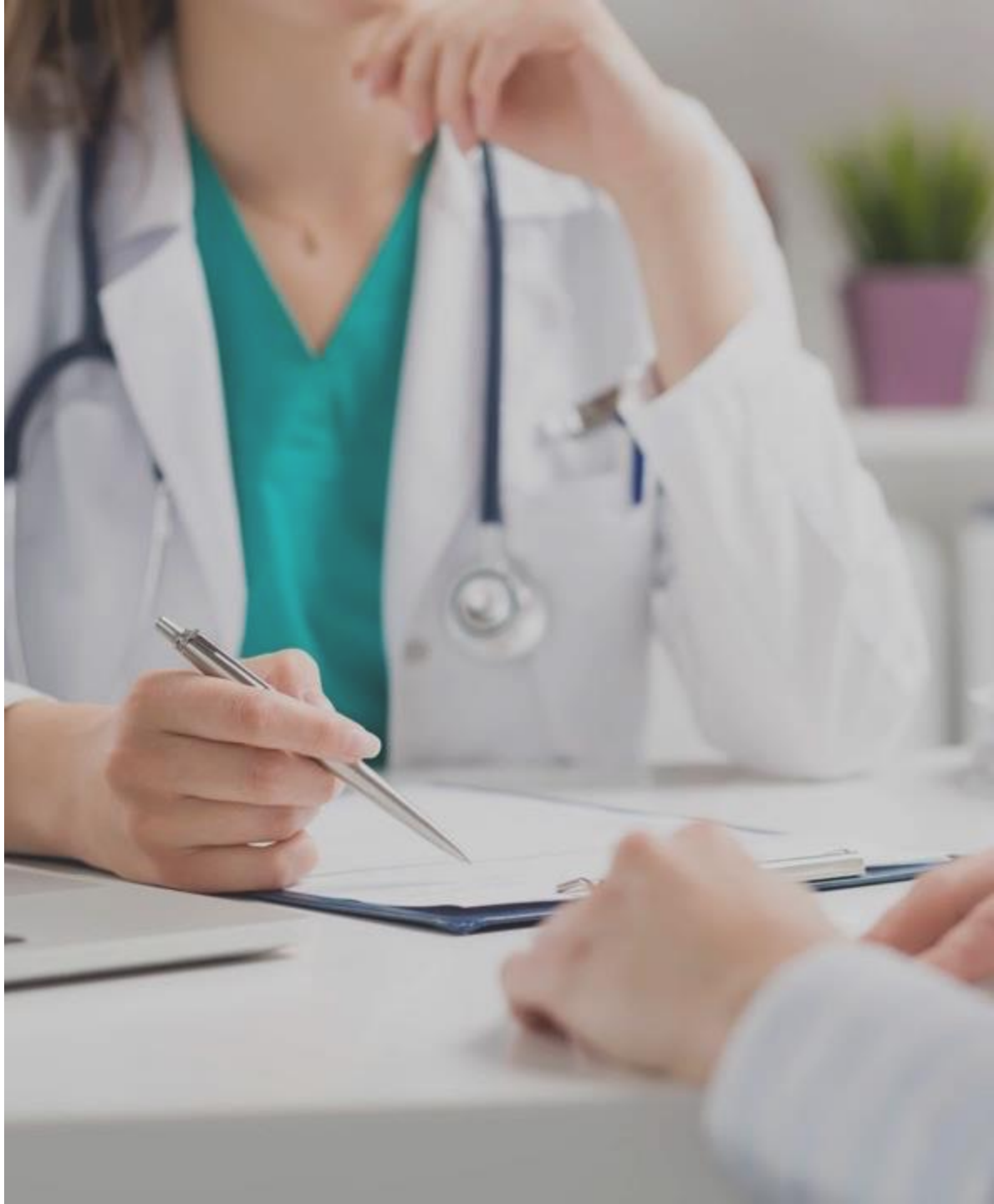
Alpine nodes

- 389 nodes in total
- 347 CPU nodes



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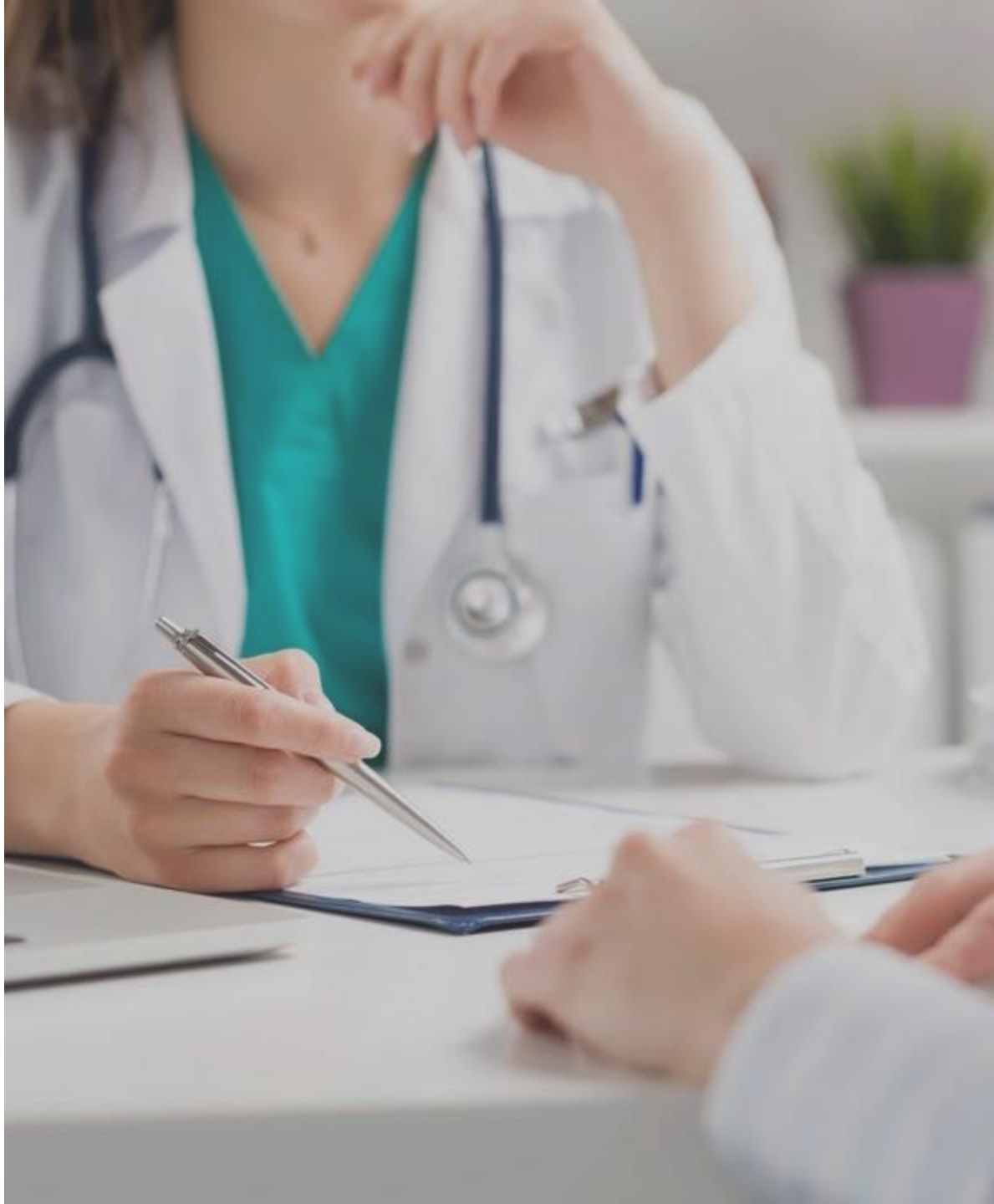
- 22 high memory nodes



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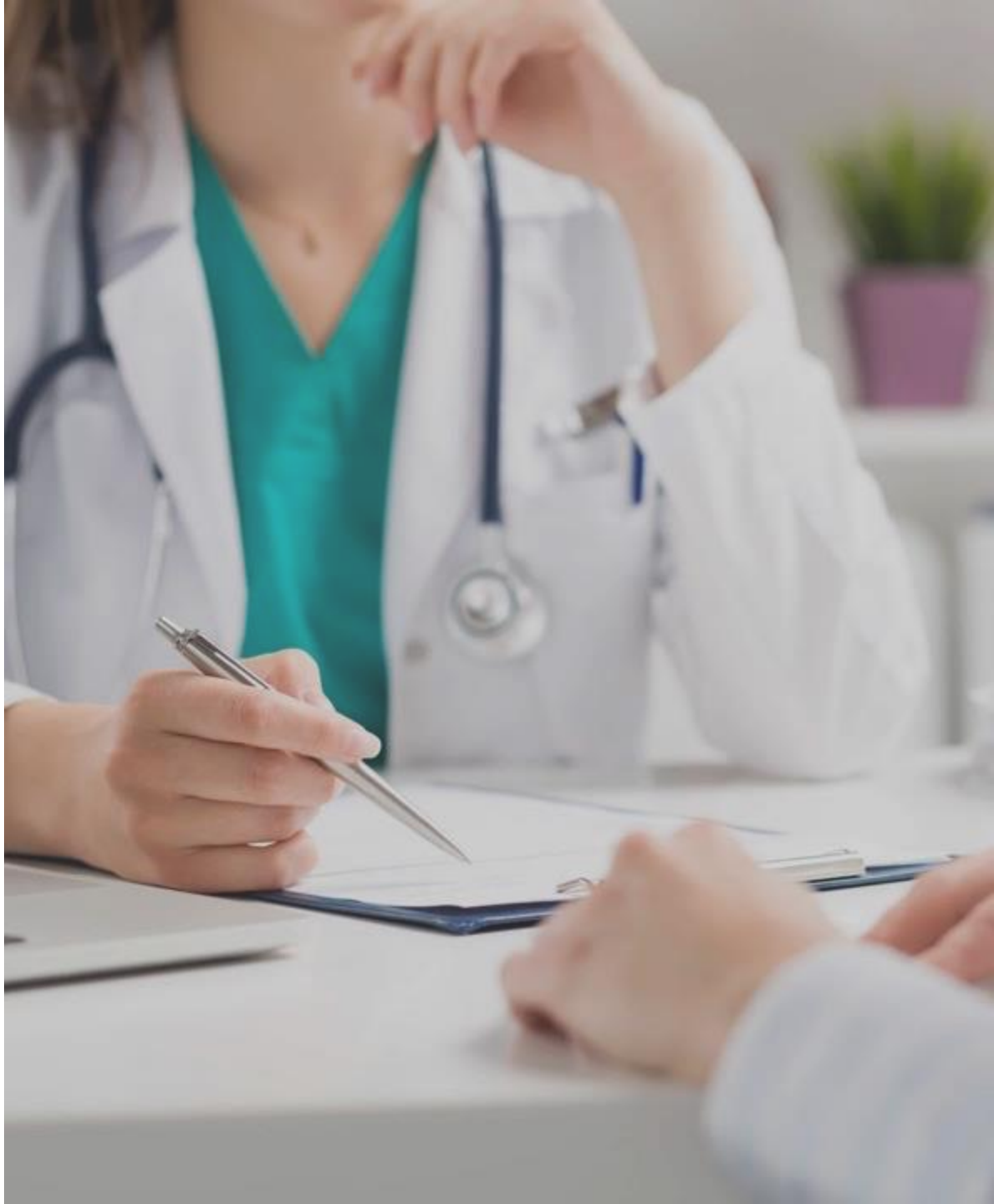
- 8 NVIDIA A100 gpu nodes (40G global mem)



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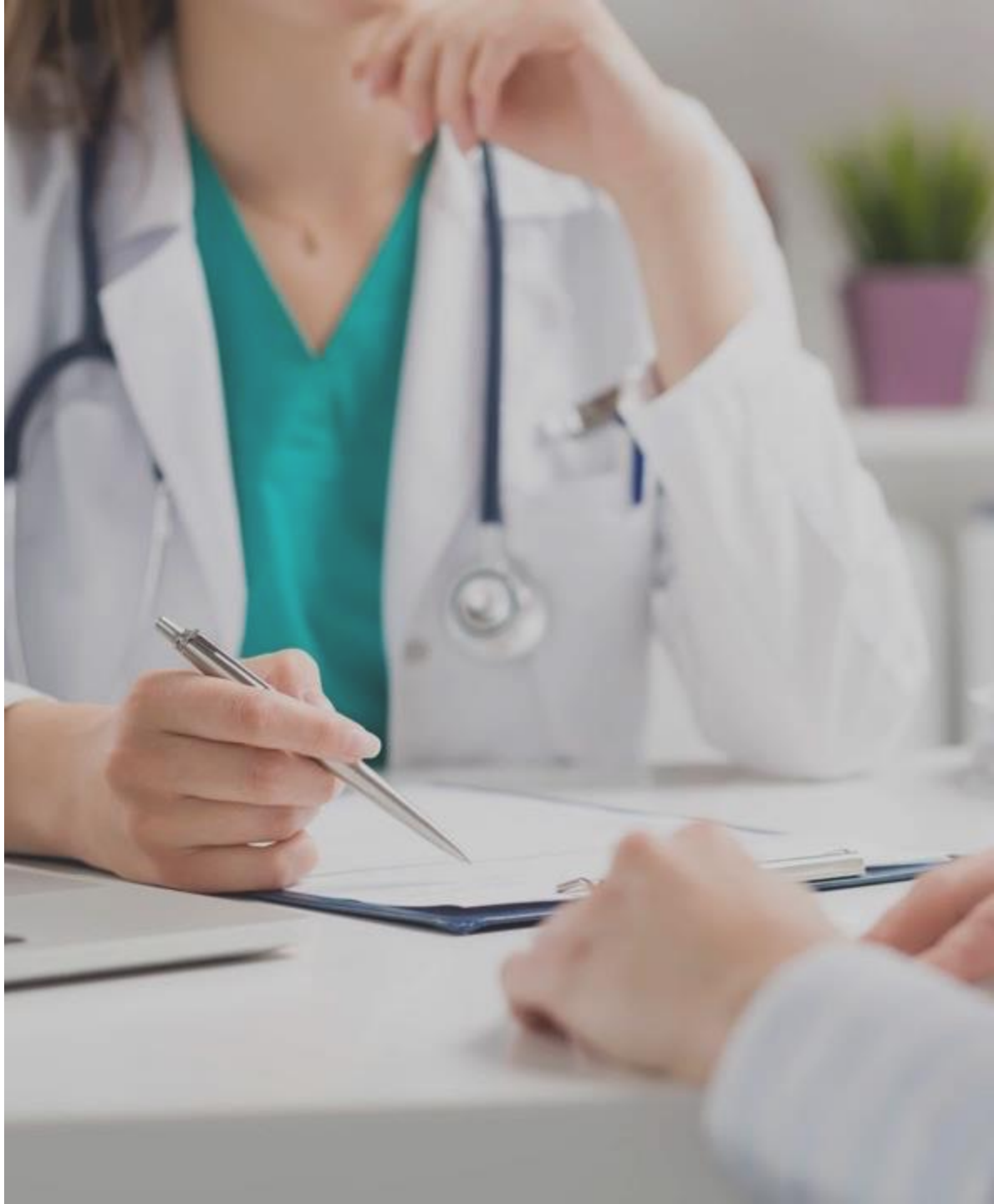

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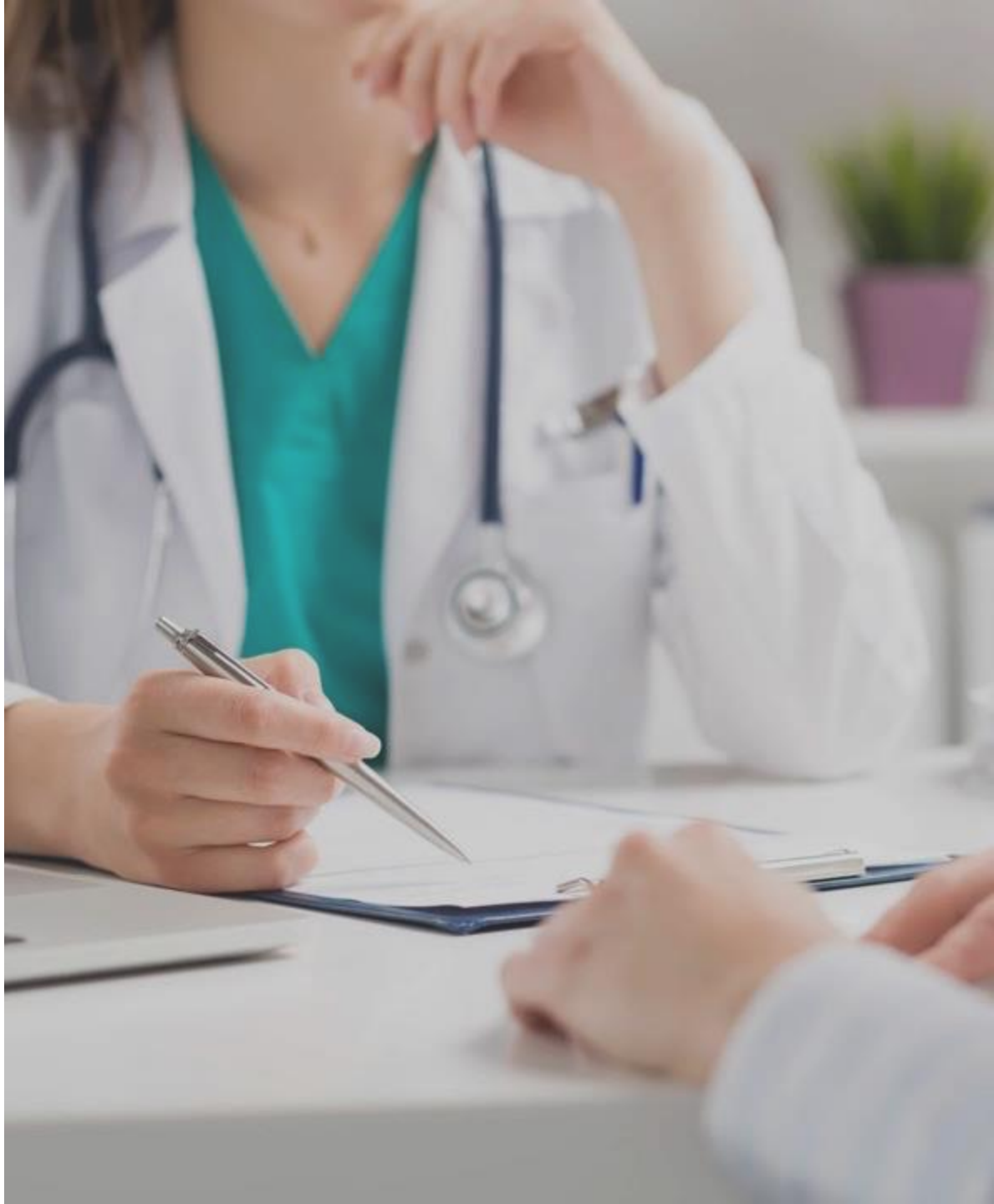

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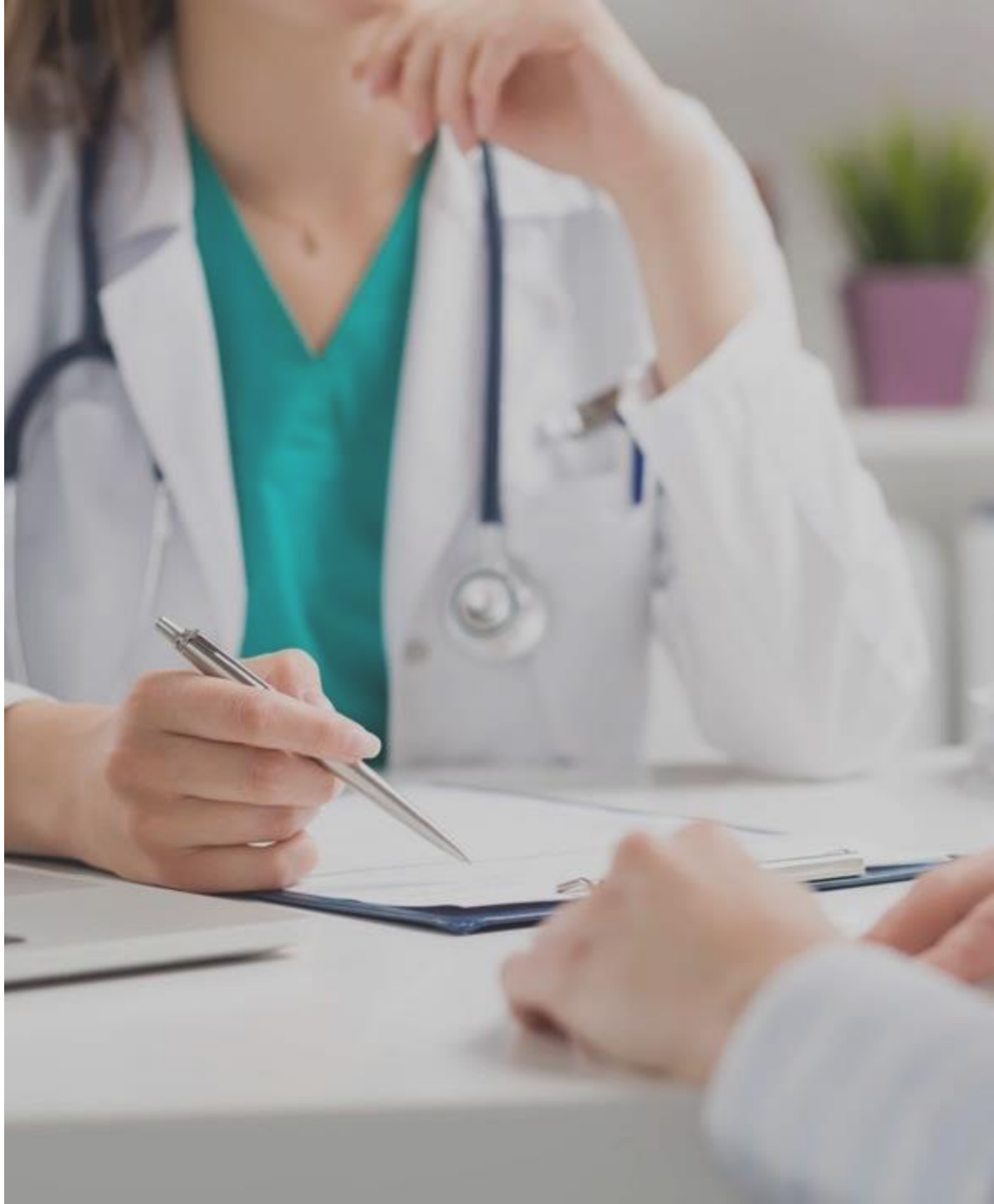
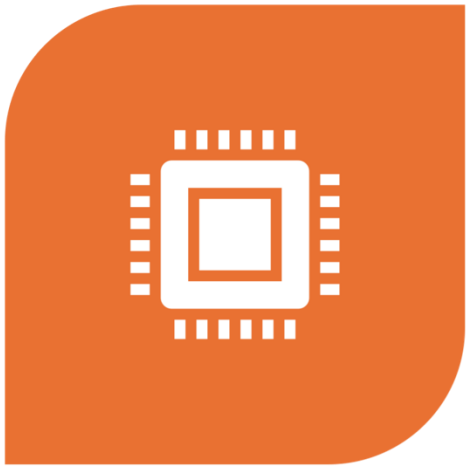
- Total of 22,180 cores



CPU nodes

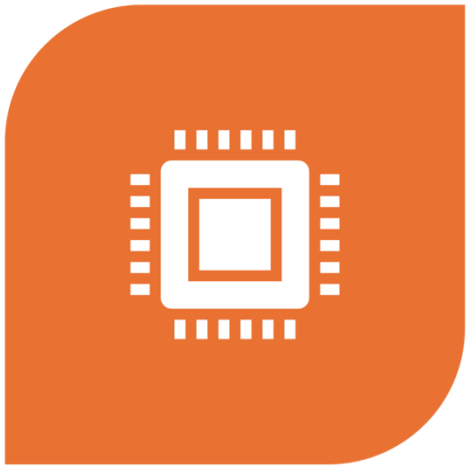
- AMD EPYC 7th generation
- 64 or 48 or 32 each
- HDR 100 Infiniband



347 CPU NODES

CPU nodes

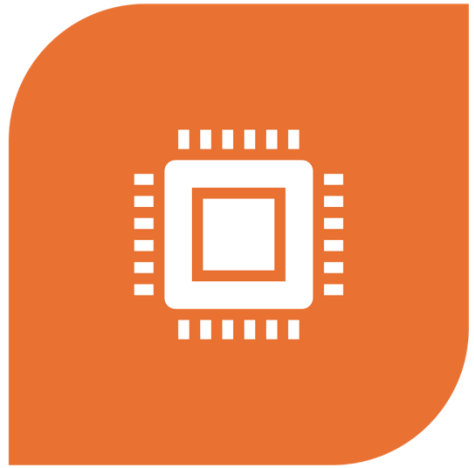
- AMD EPYC 7th generation
- 64 or 48 or 32 each
- HDR 100 Infiniband
- 240G memory



347 CPU NODES

High mem nodes nodes on Alpine

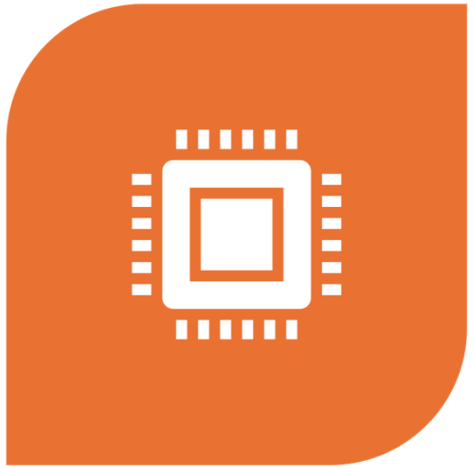
- AMD EPYC 7th generation
- 64 or 48 cores each
- 2x25 Gb Ethernet +RoCE
- Up to 1TB RAM



22 HIGH MEM NODES

NVIDIA GPU nodes on Alpine

- aa100 gpu nodes with 3Xgpus per node
- 40GB or 80GB gpu global memory
- 64 cores each
- 2x25 Gb Ethernet +RoCE



12 NVIDIA GPU NODES (3 GPU EACH)

AMD GPU nodes on Alpine

- ami100 gpu nodes with 3Xgpus per node
- 32GB gpu global memory
- 64 cores each
- 2x25 Gb Ethernet +RoCE

8 AMD GPU NODES (3 GPU EACH)

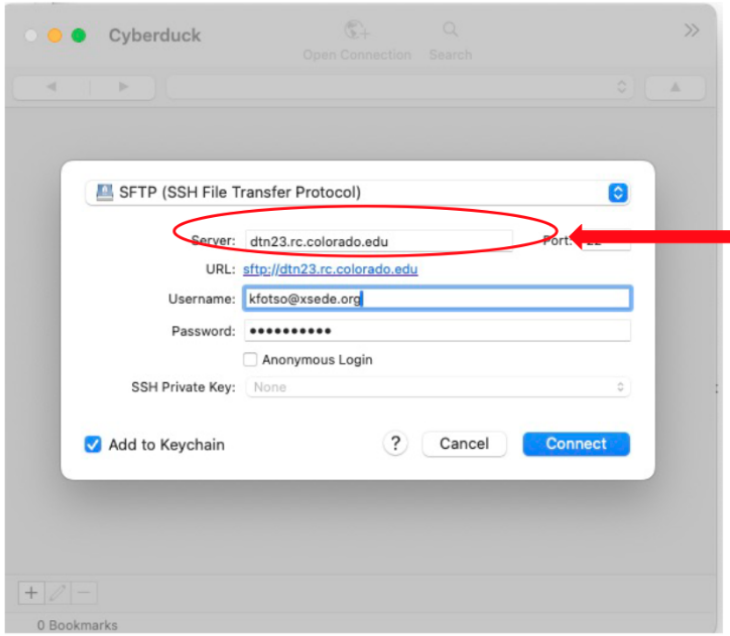
Upcoming nodes this Fall

- 12 CPU nodes
- 2X2TB high mem nodes
- NVIDIA 3XL40 gpu nodes with 3 gpus each

IV- Data transfer methods

Data transfers

- Globus, scp, rsync, sftp, cyberduck, Filezilla etc …



We point out to the Alpine data transfer node

Data transfers

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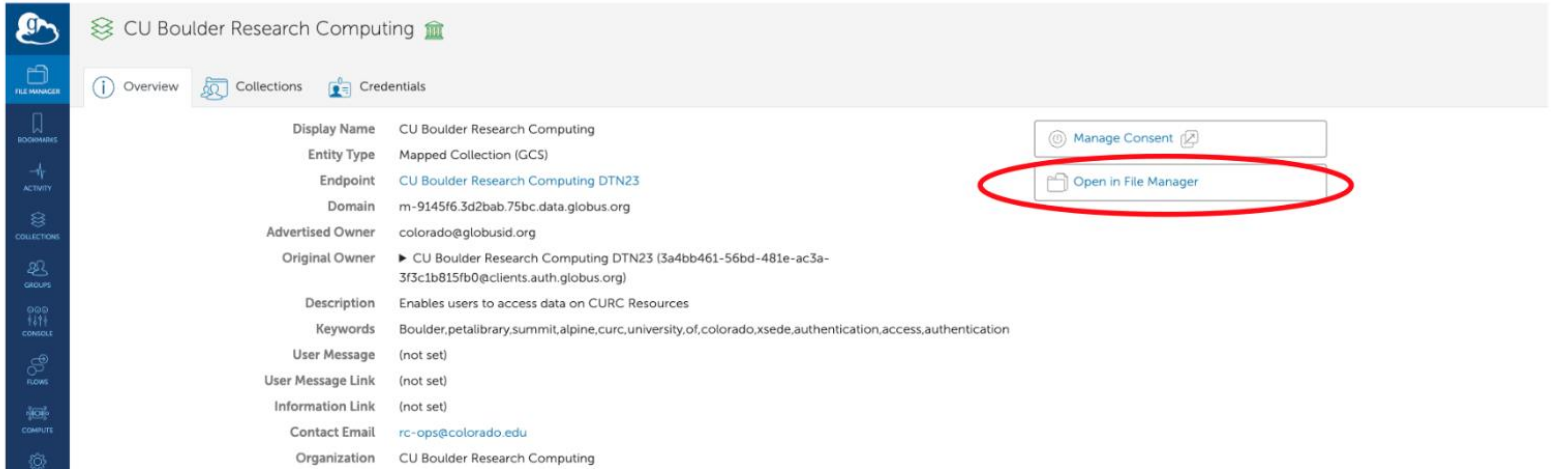

V- Alpine storage

Storage overview

- Home filesystem (2G). Backed up + for hosting config files. (free)

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Storage overview

- Home filesystem (2G). Backed up + for hosting config files. (free)
- Project filesystem (250G). Backed up -> for package installation. (free)

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- Home filesystem (2G). Backed up + for hosting config files. (free)
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- Scratch filesystem (10TB) (free)

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Storage overview

- Home filesystem (2G). Backed up + for hosting config files. (free)
- Project filesystem (250G). Backed up -> for package installation. (free)
- Scratch filesystem (10TB) (free)
- Petalibrary (optional and paid service).

Scratch overview

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

VI- Petalibrary service

What is Petalibrary?

- An Alpine service that supports the paid storage, archival, and sharing of research data.

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What is Petalibrary?

- An Alpine service that supports the paid storage, archival, and sharing of research data.
- It is available at a subsidized cost to any researcher affiliated with the University of Colorado System (Boulder, Anschutz, Denver, Colorado Springs)

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Preliminary conditions

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>
```

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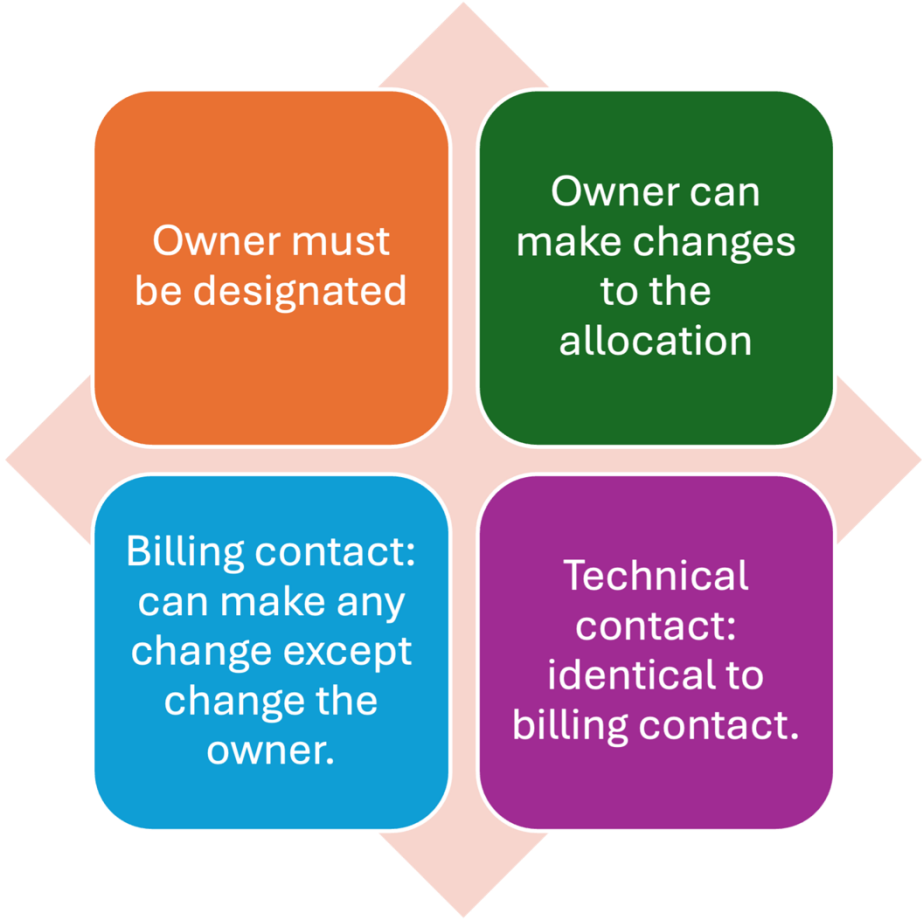
Preliminary conditions



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.

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Billing

- On active storage: $48/TB/yr.
- ZFS Raidz2 allow for frequent read/write + parity.
- It is the responsibility of the PI to estimate and foresee the PL allotment for the year.

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Billing

- On archive storage: $25/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.

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- **10,000 object (file/directory) limit.**

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- Can be accessed from RC login node only and data transfer resources.
- Min size for any alloc is 1 TB.
- **10,000 object (file/directory) limit.**
- **Owner will get and pay for the space even if they do not use it.**

Data redundancy

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

Data replication solution

- Replicated PetaLibrary active+archive allocation.
- CURC only takes data replication responsibility.

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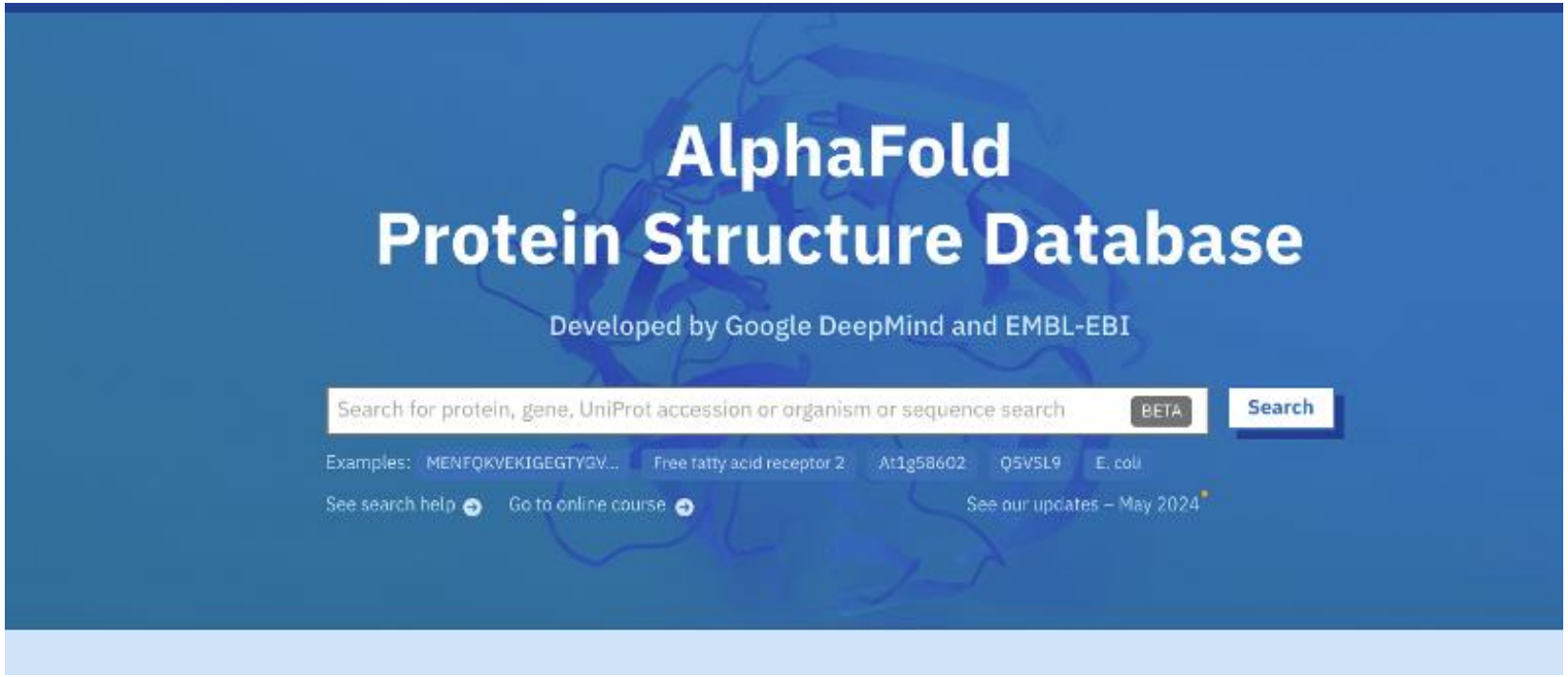
- Replicated PetaLibrary active+archive allocation.
- CURC only takes data replication responsibility.
- Not subject to the **10,000 object (file/directory) limit.**

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.
- $73/TB/year total. **(NOT $73 on top of the $48/$25 original rate!!)**

VII- Examples of HPC tools on Alpine.

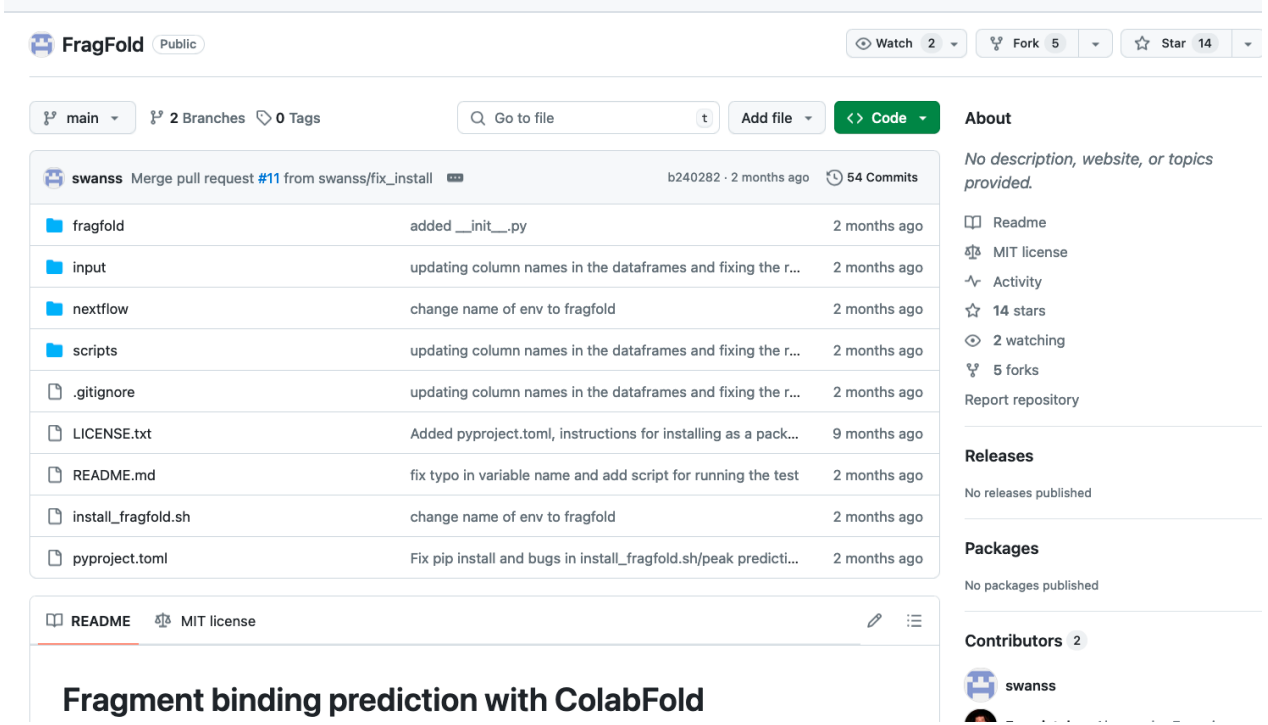
Alphafold



Source: https://alphafold.ebi.ac.uk/

Fragfold

- Fragment binding prediction
- High-throughput computational discovery of inhibitory protein fragments with AlphaFold



Source: https://www.biorxiv.org/content/10.1101/2023.12.19.572389v1 ; https://github.com/swanss/FragFold;

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Containers

- Apptainer/Singularity can now be built directly on the cluster
- Can be built either from a definition file or converted from a docker image.

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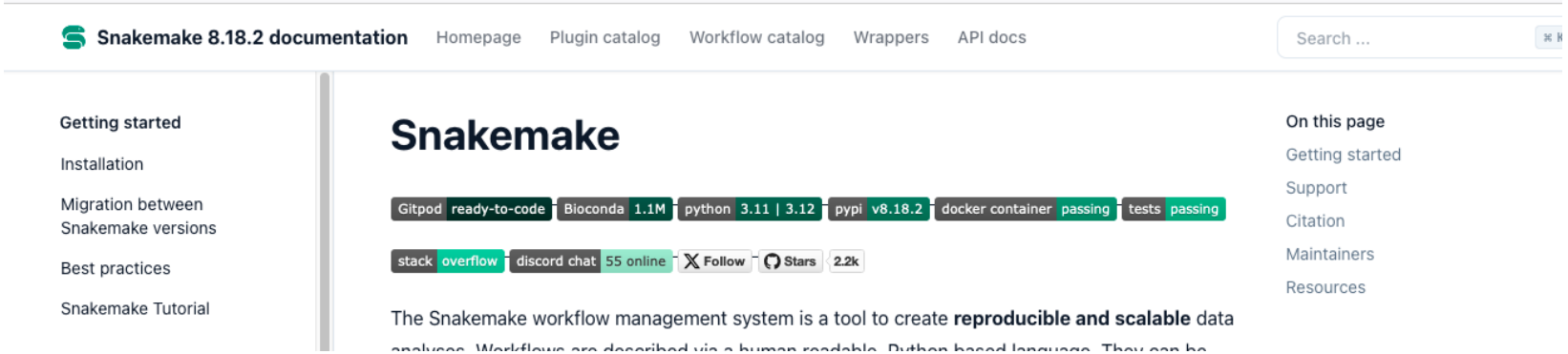
- Apptainer/Singularity can now be built directly on the cluster
- Can be built either from a definition file or converted from a docker image.
- Available on all compute nodes.
- e.g: **apptainer build horovod_cuda.sif docker://horovod/horovod:latest**

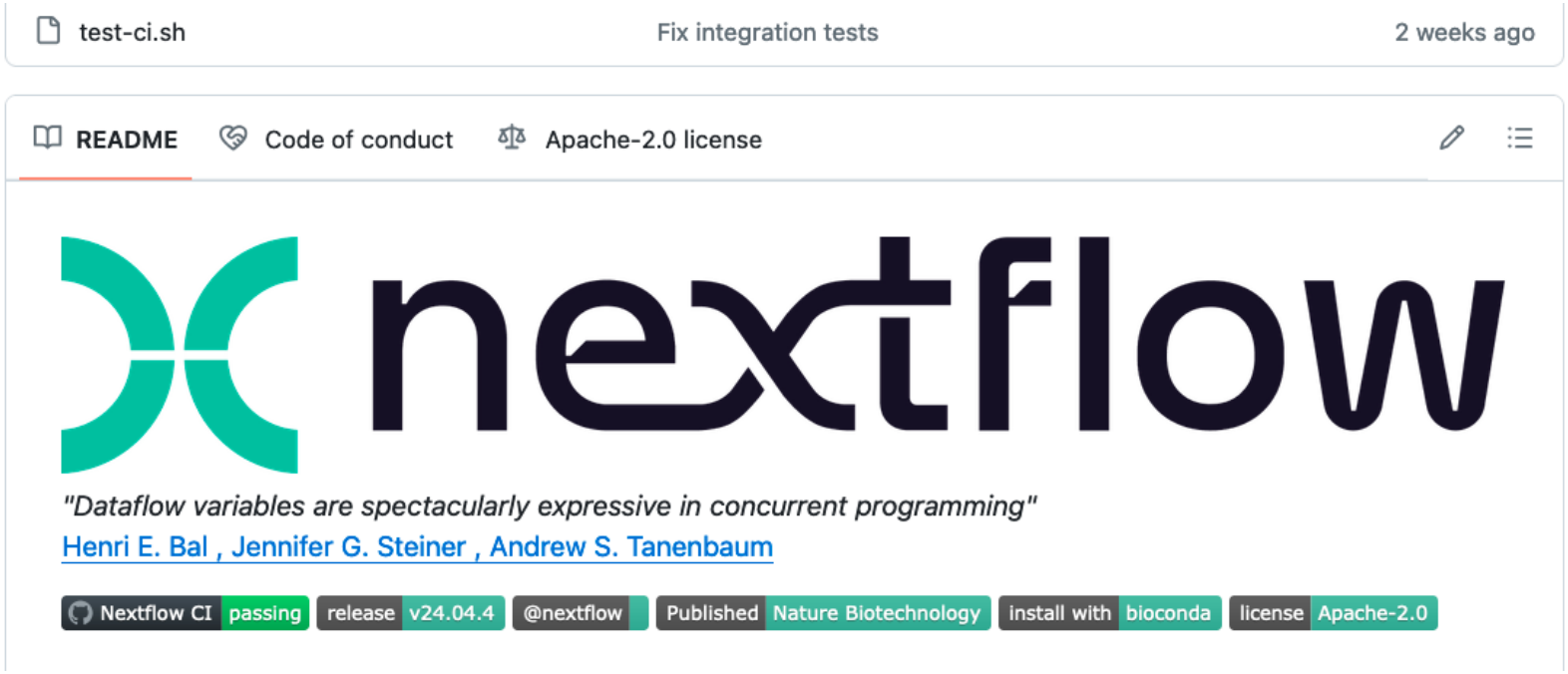
Snakemake



- Workflow management software compatible with slurm

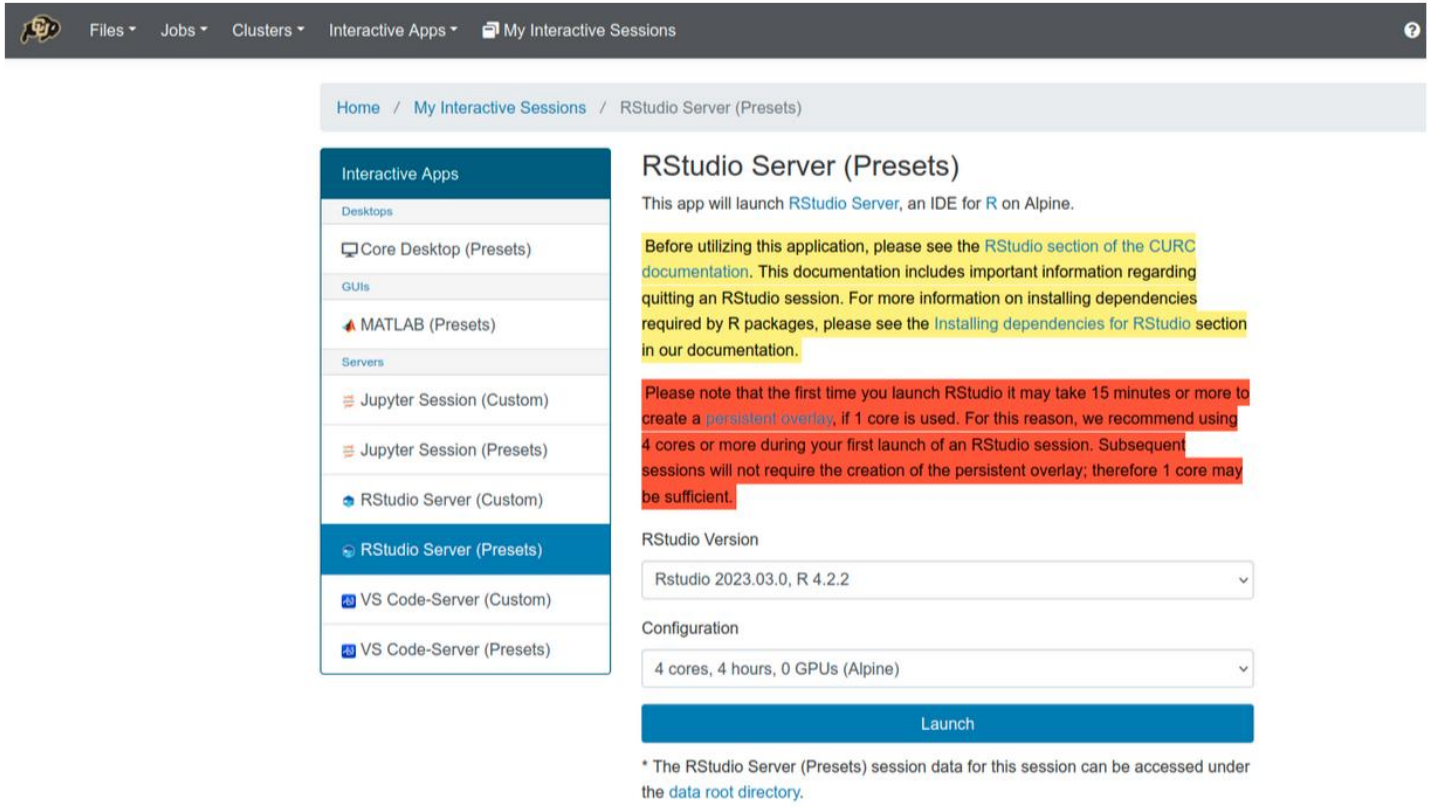
Source: https://snakemake.readthedocs.io/en/stable/

Nextflow



Source: https://github.com/nextflow-io/nextflow

Rstudio instances

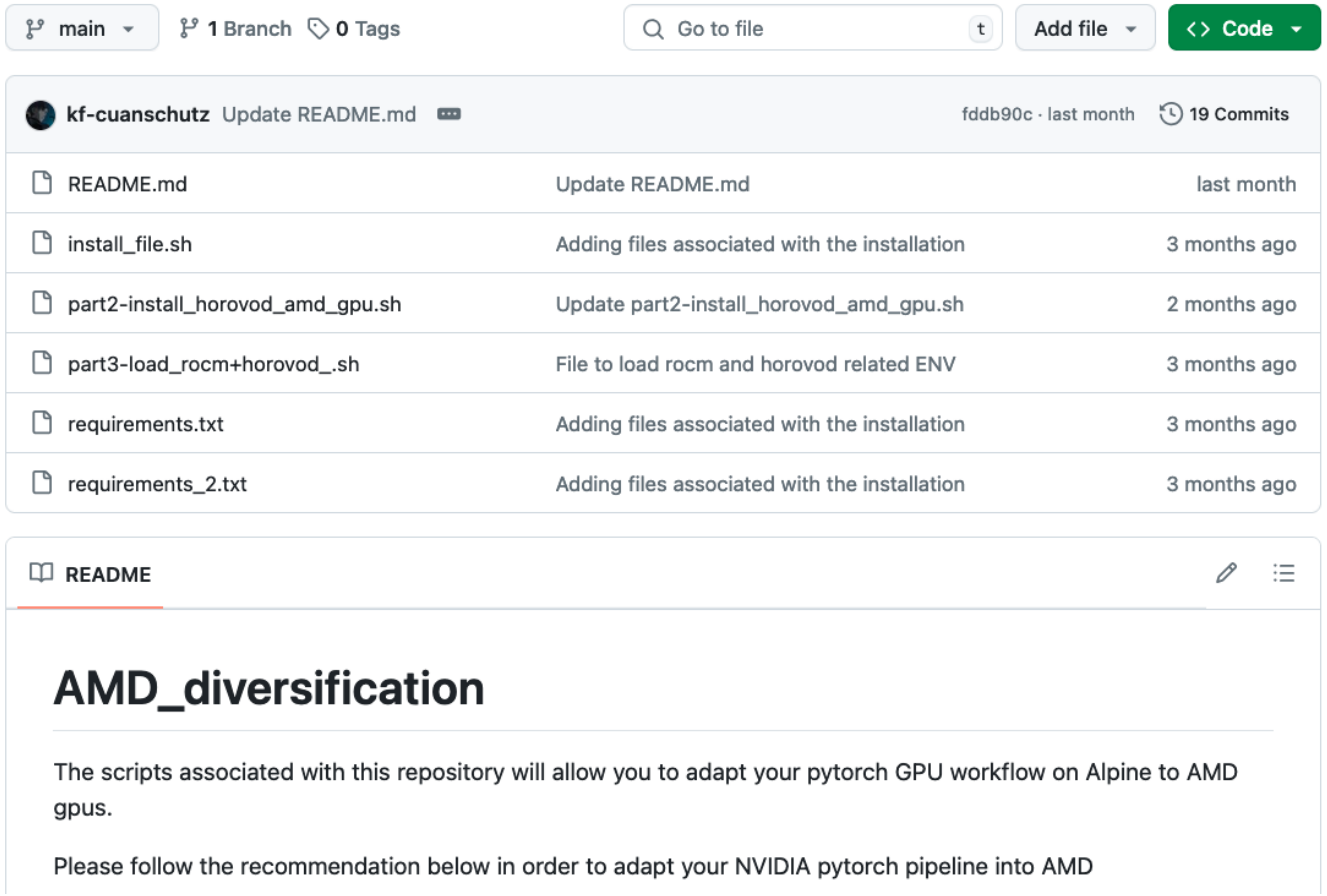


- Dedicated Rstudio, Vscode, MATLAB or Jupyterlab instances.

Source:https://github.com/kf-cuanschutz/CU-Anschutz-HPC-documentation/tree/main/Rstudio_related_scripts

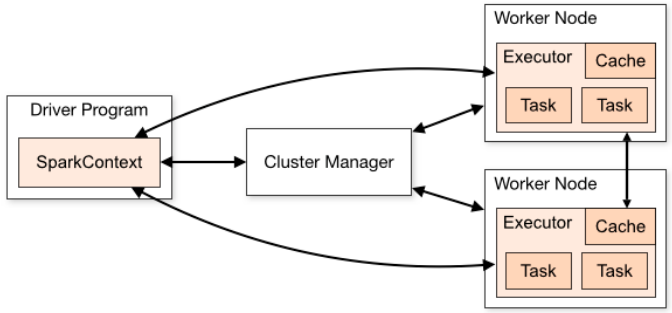
Distributed deep learning on multiple nodes

- Horovod on both NVIDIA & AMD gpus support



Source:https://github.com/kf-cuanschutz/AMD_diversification/tree/main

Hail & Sparcluster distributed computing




```
# Loading the hail module
module load hail

# We want the name of the nodes we requested
scontrol show hostname > $SLURM_SUBMIT_DIR/nodelist.txt
export SLURM_NODEFILE=$SLURM_SUBMIT_DIR/nodelist.txt

# We submit hail with the custom made slurm-spark-submit which was modified from: https://lobogit.unm.edu/CARC/tutorials/-/blob/master/spark/pbs-spark-submit
# The hail script was modified from https://hail.is/docs/0.2/install/other-cluster.html
#
python slurm-spark-submit \
--jars $HAIL_HOME/backend/hail-all-spark.jar \
--conf spark.driver.extraClassPath=$HAIL_HOME/backend/hail-all-spark.jar \
--conf spark.executor.extraClassPath=./hail-all-spark.jar \
--conf spark.serializer=org.apache.spark.serializer.KryoSerializer \
--conf spark.kryo.registrator=is.hail.kryo.HailKryoRegistrator hail-script.py --temp_dir $TMP
```

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Source:https://github.com/kf-cuanschutz/Hail_support_cu_anschutz

Jobs in chain and job arrays with slurm

```
# Adressing the total number of files to be processed
actual_work_files=$(< "$scripts_dir/files_to_process.txt" wc -l)
total_work_files=$(( actual_work_files*2 ))

# Phase 1 FastQC Raw, no dependencies:
#  Note: Job arrays have been added for that step.

# Producing the files to be processed for phase 1
ls $base_dir/Raw_Sequences/NW_*.fastq.gz > arg_fastq_raw_tmp.txt
sort arg_fastq_raw_tmp.txt | uniq -u > arg_fastq_raw.txt

tmp1=$(sbatch --array=1-$total_work_files ${scripts_dir}/FastQC_Raw.sh $base_dir)
jid1=`echo ${tmp1##* }`

# Setting up sbatch to avoid dependency error
alias sbatch='sbatch --export=NONE'

# Phase 2 Skewer_trim, dependency jid1
# RAW_DIR="/scratch/alpine/                    /SEARCH-TB_base_dir/Raw_Sequences"
# num_skewer_files=$(< "$RAW_DIR/arg_skewer_trim.txt" wc -l)
tmp2=$(sbatch --array=1-$total_work_files --dependency=afterany:$jid1 $scripts_dir/Skewer_trim.sh $base_dir)
```

Bioinformatics modules on Alpine

```
--------------------
alphafold/2.2.0
alphafold/2.3.1 (D)
bamtools/2.5.2

--------------------
 samtools/1.16.1
 sra-toolkit/3.0.0
 star/2.7.10b

plink2/2.00a2.3
qiime2/2023.5
qiime2/2024.2_amplicon
```

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 star/2.7.10b

plink2/2.00a2.3
qiime2/2023.5
qiime2/2024.2_amplicon
```

```
------------------
  cutadapt/4.2
  fastqc/0.11.9
  gatk/4.3.0.0

------------------
 bowtie2/2.5.0
 bwa/0.7.17
 cellranger/7.1.0

nextflow/22.10.6
nextflow/23.04
picard/2.27.5
```

Bioinformatics modules on Alpine

```
alphafold/2.2.0
alphafold/2.3.1 (D)
bamtools/2.5.2
```

```
cutadapt/4.2
fastqc/0.11.9
gatk/4.3.0.0
```

```
bbtools/39.01
bcftools/1.16
bedtools/2.29.1
```

```
samtools/1.16.1
sra-toolkit/3.0.0
star/2.7.10b
```

```
bowtie2/2.5.0
bwa/0.7.17
cellranger/7.1.0
```

```
homer/4.11
htslib/1.16
multiqc/1.14
```

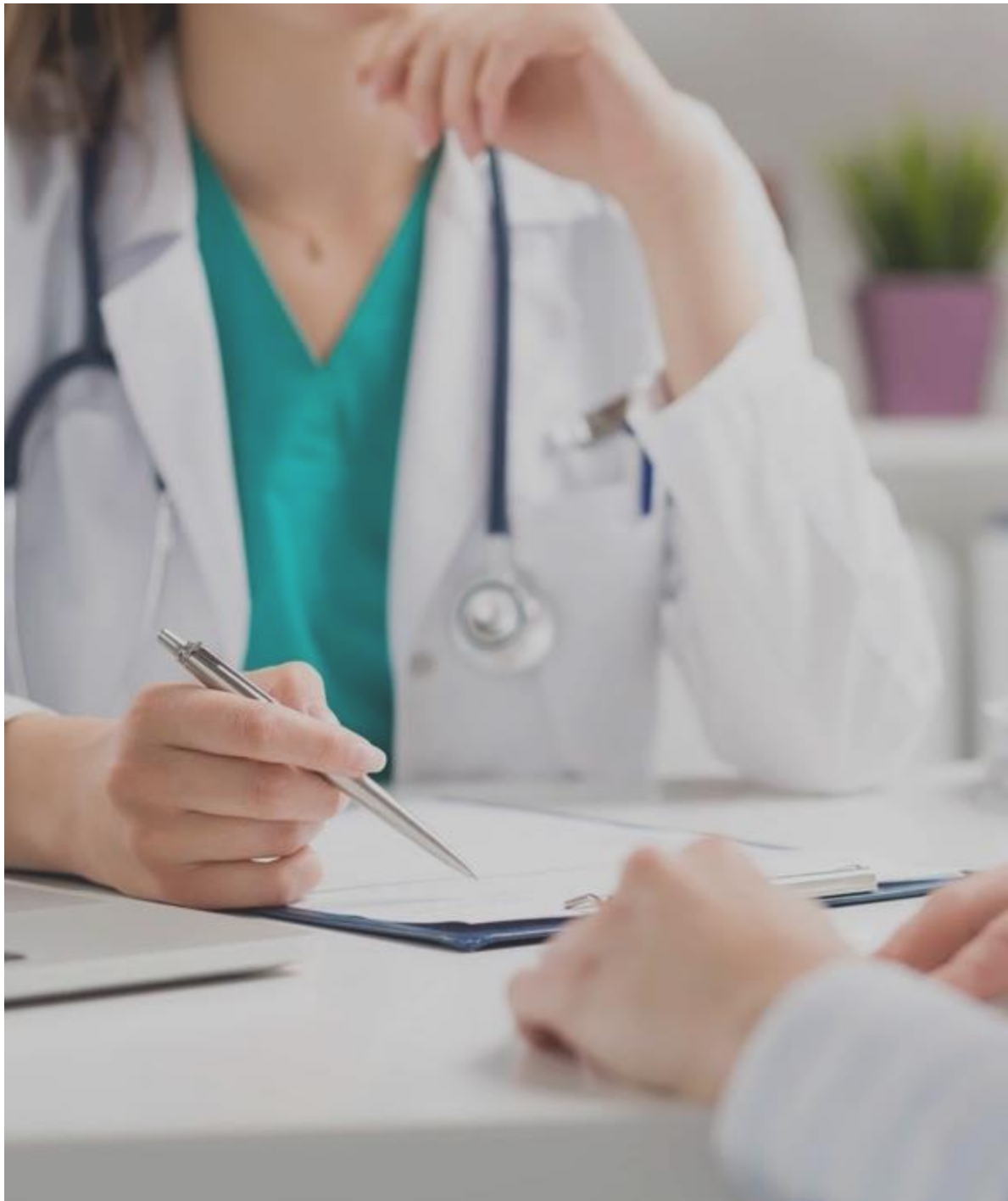
```
plink2/2.00a2.3
qiime2/2023.5
qiime2/2024.2_amplicon
```

```
nextflow/22.10.6
nextflow/23.04
picard/2.27.5
```

```
trimmomatic/0.39
```

Many more …

- We will work with you to build any publicly available module not discussed here.



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VIII- Workshops

Workshops

- On many aspects of Research computing (Introduction to the cluster, Deep learning, parallel computing, Package installation etc …)

VI- Lab workshops:

Workshops given to customized to labs that have been already given. Send an email to rc-help@colorado.edu to request a workshop.

- List of workshops:
  - NVIDIA Mark III Sys workshop series (05/04/23 to 06/22/23). Additional information can be found here.
  - Introduction to the Shell - Barocas lab
  - Introduction to Slurm - Barocas lab
  - Introduction to Alpine - Kalpathy-Cramer lab
  - Introduction to Slurm and Petalibrary - Lange lab
  - GPU partitions on Alpine Janani lab 090623
  - Alpine entry level workshop 090723
  - Immuno 6110 class 090723
  - Intro to spack part 1 10/17/23
  - Intro to Horovod part 1 10/24/23
  - Alpine entry level workshop 110223
  - Intro to GPU computing part 1 112823
  - Intro to GPU computing part 2 113023
  - Intro to GPU computing part 3 120423
  - Alpine for noobs workshop 120723
  - AMD_GPU_computing_022924
  - Alpine_entry_level_workshop_030524
  - NVIDIA Mark III Sys workshop series Spring 2024 (01/25/24 to 05/02/24)

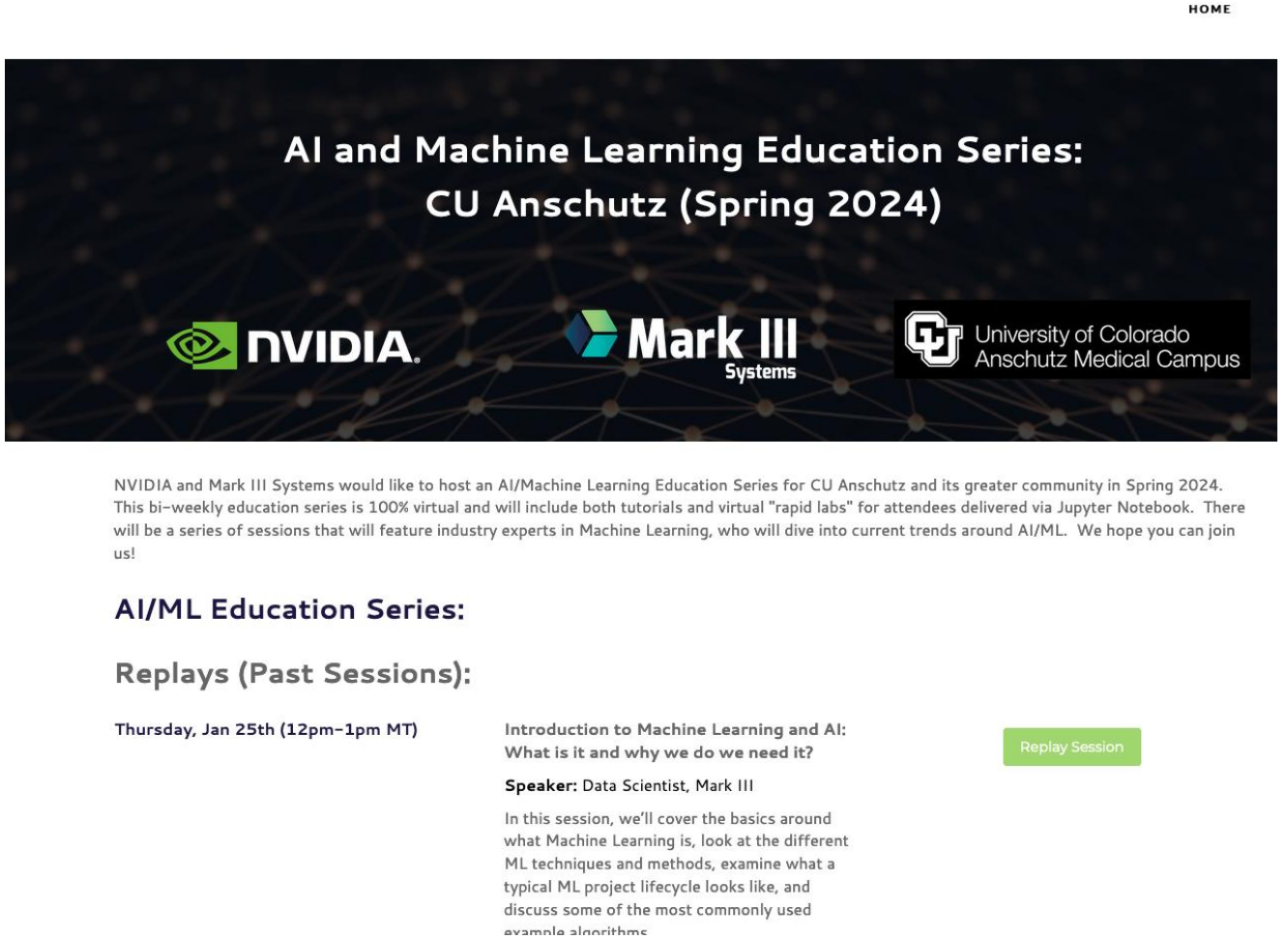
1st workshop to get started

2nd workshop to get started

Source:https://github.com/kf-cuanschutz/CU-Anschutz-HPC-documentation/tree/main

Workshops

- NVIDIA collaborations with trainings in bioinformatics, Machine learning, containers, and LLMs.



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Source: https://trending.markiiisys.com/cu-anschutz-ai-2024

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THANK YOU