Northwestern
INFORMATION TECHNOLOGY

# A Quest for Computing at Northwestern

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# Computing environments

## A typical desktop/laptop

- Local access
- A single "node"
- Windows, MacOS, maybe Linux
- Limited to the hardware *you* can afford
- Lower RAM (4-16GB), lower core count (4-12), likely an integrated GPU
- Easy to use!

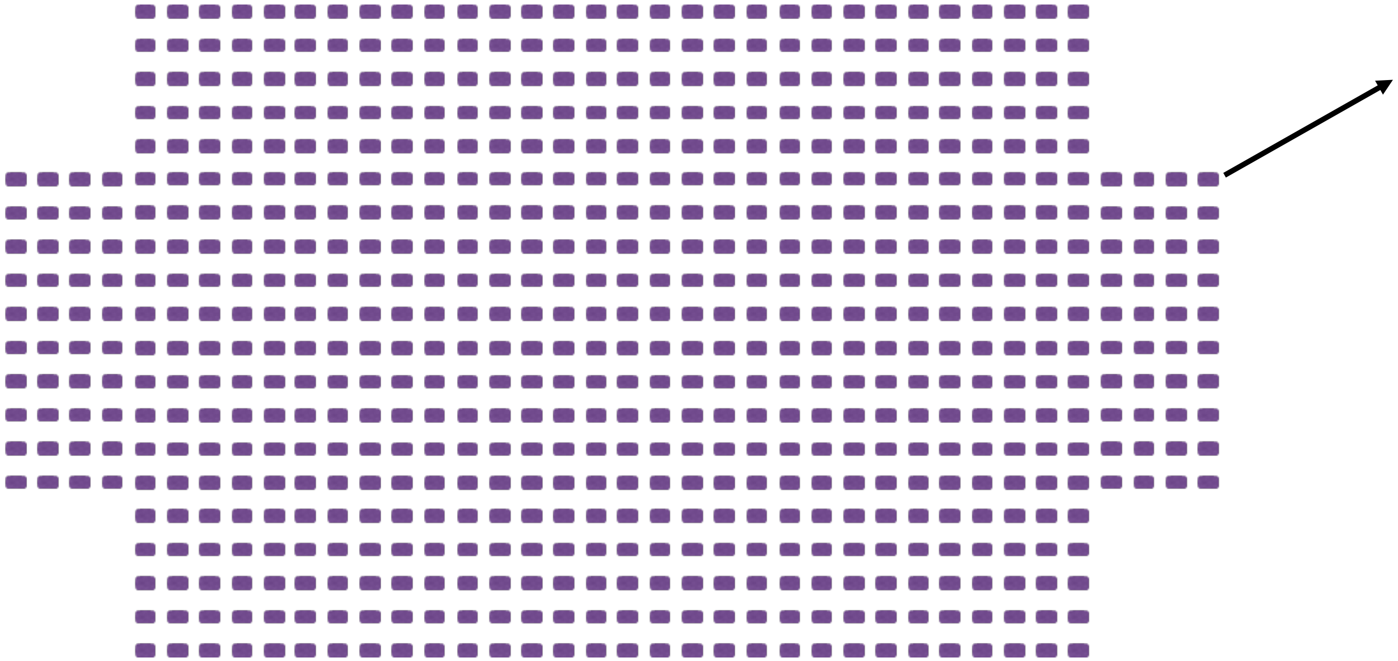
## A "cluster"

- Remote access
- Many "nodes"
- Almost certainly Linux
- Limited to the hardware *a large institution* can afford ($$$)
- Higher RAM (up to 1.5TB), higher core count (52+), dedicated GPU resources
- Takes time to learn!

# What is Quest?

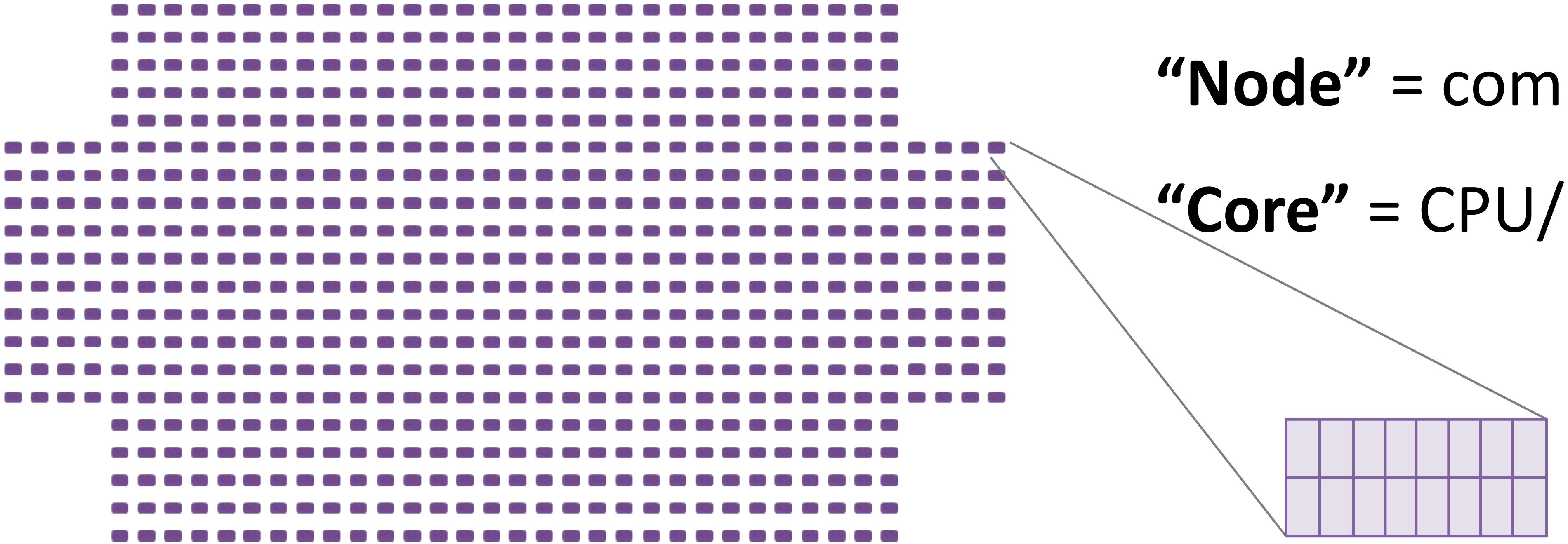
# Quest: Northwestern's High-Performance Computing Cluster

# Quest consists of ~1000 nodes



**“Node”** = computer

# Each node consists of 28-64 cores

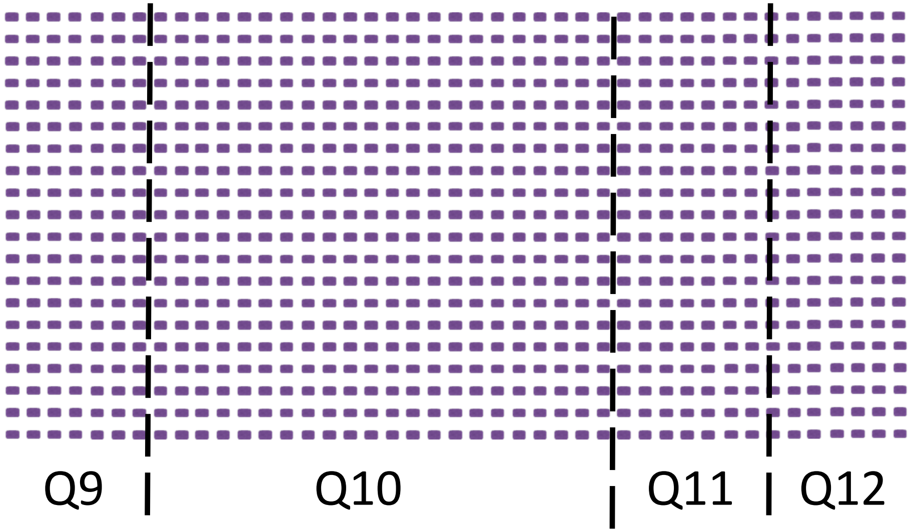


**"Node"** = computer

**"Core"** = CPU/processor

# Technical specifications of nodes vary

There are several generations of nodes!



| Generation | # cores per node | Total memory | Memory per core |
|---|---|---|---|
| Q9 | 40 | 192 GB | ~4.8 GB |
| Q10 | 52 | 192 GB | ~3.7 GB |
| Q11 | 64 | 256GB | ~4GB |
| Q12 | 64 | 256GB | ~4GB |

# Other types of nodes available for “General Access” (i.e., free) use

- “General Access”
  - 15 A100 GPU nodes
    - 40GB RAM (PCIE)
    - 80GB RAM (SXM)
  - 1 high memory node
    - 1.5TB RAM

https://www.nvidia.com/en-us/data-center/a100/

# Extra resources for bioinformaticians at NU

- The "Genomics Compute Cluster" (GCC)
  - A special account funded by Feinberg & Weinberg to support bioinformatics/genomics research at NU
- 8 additional A100 GPU cards on 2 nodes
- 3 additional high memory nodes with RAM up to 1.5TB
- ~350TB of shared scratch space
- Dedicated support specialist: **Haley Carter**

Learn more about the GCC!

# Quest Analytics Nodes

The Quest Analytics Nodes provide…

- On-demand access to Rstudio Server, Jupyter and SAS Studio through the web browser.
- Access to Quest file system.
- More computational resources than available on a personal computer.

The Quest Analytics Nodes are…

- Available to all Quest users with an active allocation
- Accessible while on GlobalProtect VPN outside the campus

[Learn more about Quest Analytics Nodes]

# How can I start using Quest?

# Apply for a general access allocation

## Research I Allocation

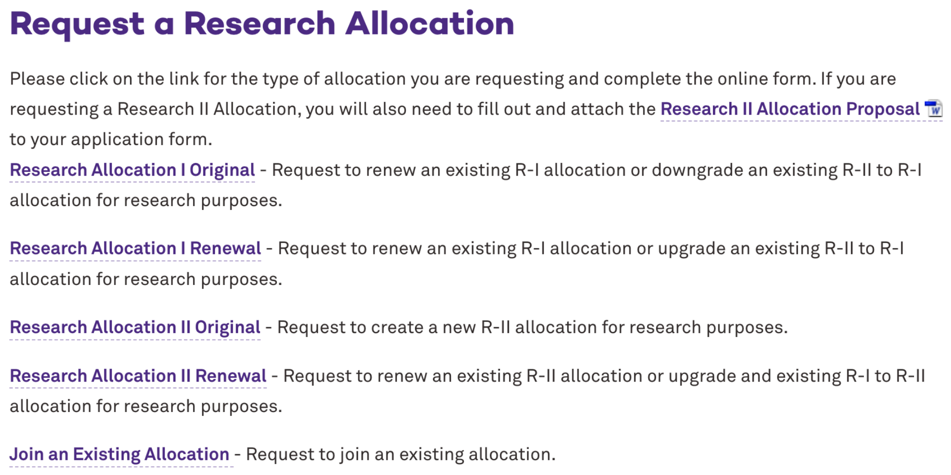
- 1 paragraph statement of purpose
- Approval process within 5 business days
- Renew for allocation yearly

## Research II Allocation

- Research I allocations can be upgraded to Research II allocations via Research II renewal form
- **Requires a research proposal**

## Join the Genomics Compute Cluster!

- Join allocation "b1042"



### Request a Research Allocation

Please click on the link for the type of allocation you are requesting and complete the online form. If you are requesting a Research II Allocation, you will also need to fill out and attach the Research II Allocation Proposal to your application form.

Research Allocation I Original - Request to renew an existing R-I allocation or downgrade an existing R-II to R-I allocation for research purposes.

Research Allocation I Renewal - Request to renew an existing R-I allocation or upgrade an existing R-II to R-I allocation for research purposes.

Research Allocation II Original - Request to create a new R-II allocation for research purposes.

Research Allocation II Renewal - Request to renew an existing R-II allocation or upgrade and existing R-I to R-II allocation for research purposes.

Join an Existing Allocation - Request to join an existing allocation.

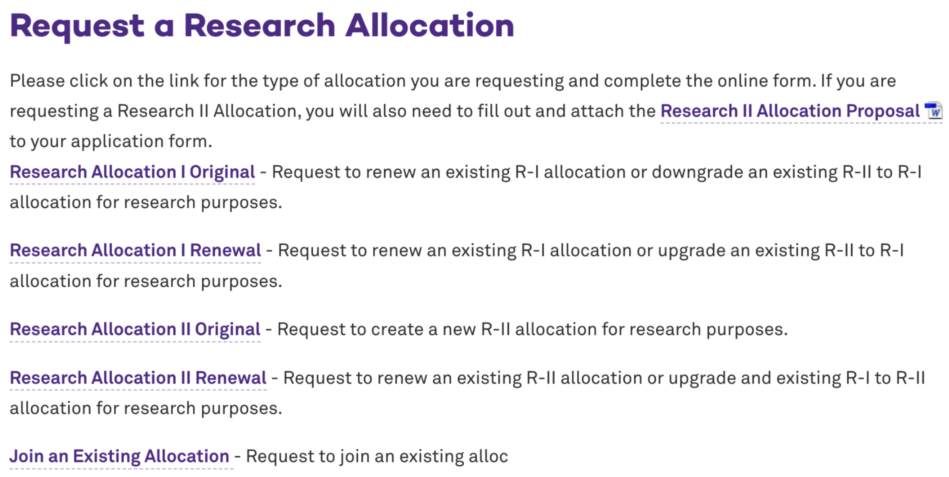
Apply now!

General access allocations are totally free to use

# Purchasing resources on Quest

- “Buy-in” allocations are a great option for faculty wanting dedicated compute/storage on Quest
- Resources purchased for a period of 5 years

- Contact us if you are interested!



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Join an Existing Allocation - Request to join an existing alloc

More information about buy-in allocations

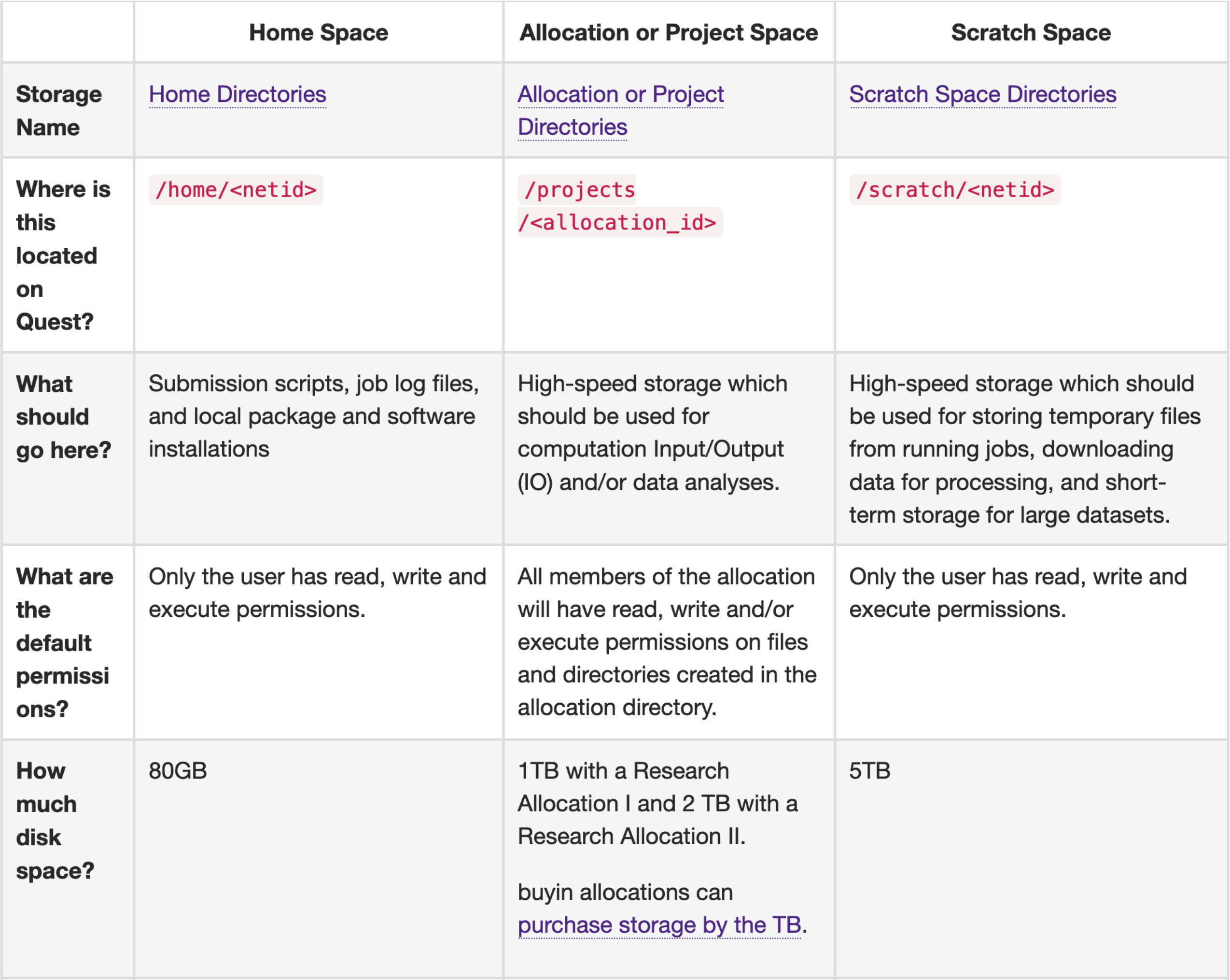
# Quest's filesystem

- **File system is shared across all computers on Quest**
  - You can access your files & folders from anywhere – you do not have to be on the same node
- **You will be working with 4 main folders:**

| Folder | Description | Space |
|---|---|---|
| /home/<netID> | Personal home directory | 80GB |
| /projects/<allocID> | Allocation directory | 1TB (R1) or 2TB (R2) |
| /scratch/<netID> | Scratch space (opt-in) | 5TB |
| /hpc/software | System-level software | N/A |

# Quest's filesystem: extra resources

- Quest Storage Knowledge Base
- Quest Storage and Data Policy



| | Home Space | Allocation or Project Space | Scratch Space |
|---|---|---|---|
| Storage Name | Home Directories | Allocation or Project Directories | Scratch Space Directories |
| Where is this located on Quest? | `/home/<netid>` | `/projects/<allocation_id>` | `/scratch/<netid>` |
| What should go here? | Submission scripts, job log files, and local package and software installations | High-speed storage which should be used for computation Input/Output (IO) and/or data analyses. | High-speed storage which should be used for storing temporary files from running jobs, downloading data for processing, and short-term storage for large datasets. |
| What are the default permissions? | Only the user has read, write and execute permissions. | All members of the allocation will have read, write and/or execute permissions on files and directories created in the allocation directory. | Only the user has read, write and execute permissions. |
| How much disk space? | 80GB | 1TB with a Research Allocation I and 2 TB with a Research Allocation II.<br>buyin allocations can purchase storage by the TB. | 5TB |

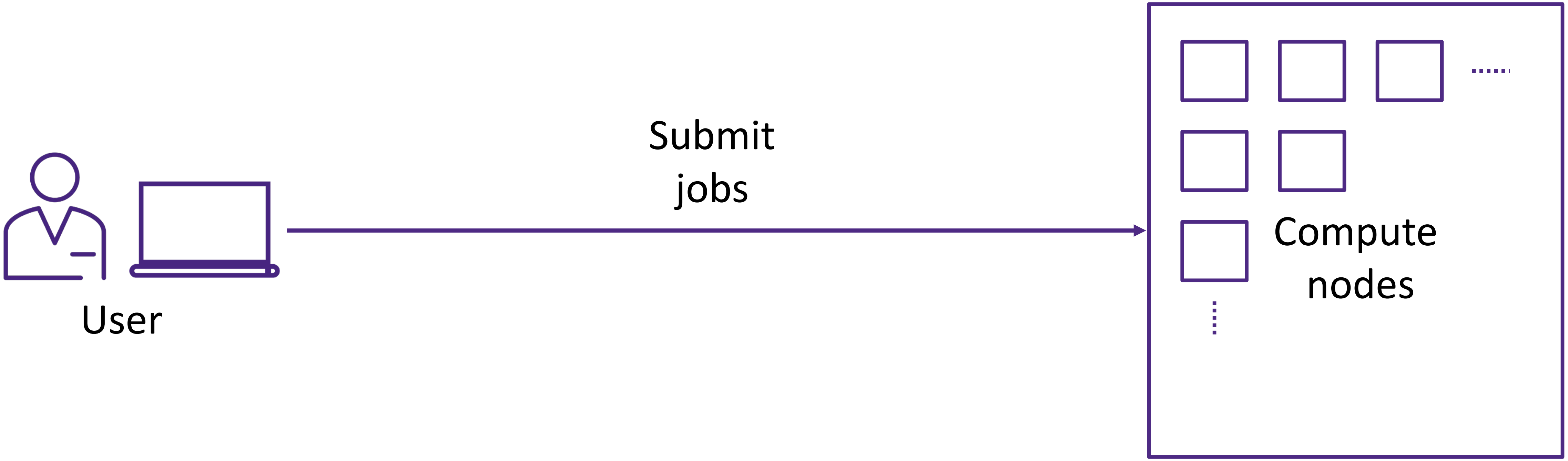
# Transferring data to and from Quest: Globus

- Globus transfers have faster rates compared to `scp`, `rsync` or `sftp`.
- Globus enables collaboration and data sharing on local or remote systems
- "Fire and forget" transfers, retries any failed attempts, checks for corruption
- [Learn more about Globus!]()

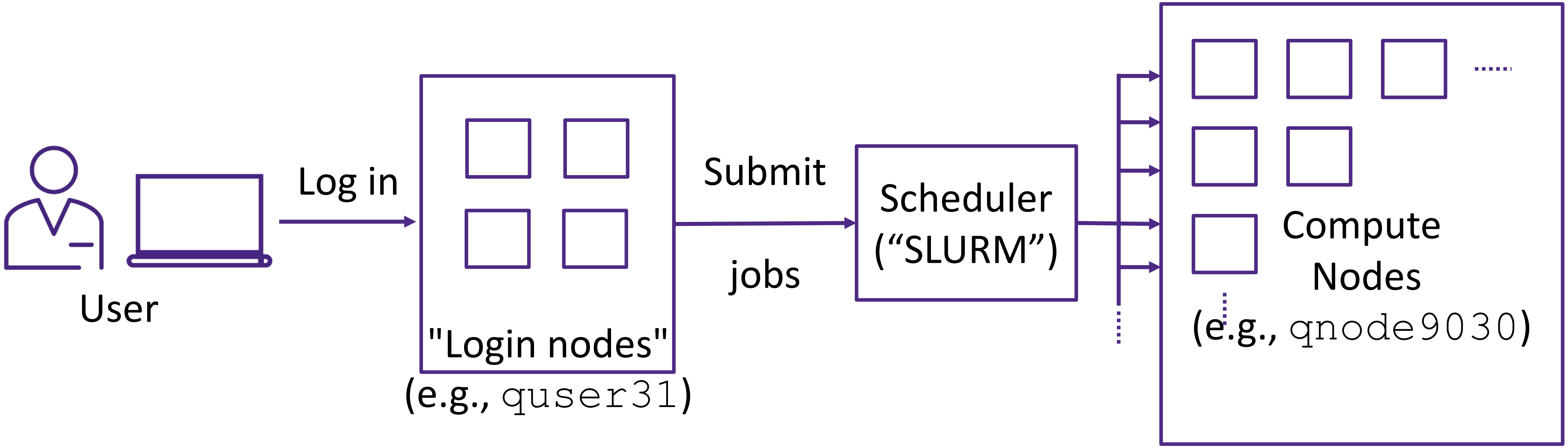
10 Years of Connecting the Research Universe

Research data management simplified.

# Submitting jobs to the Quest compute nodes



# Log into the login nodes & submit jobs to the scheduler



# *Jobs*: Requesting resources from SLURM

- **Batch job**
  - ○ Submit your job as a pre-written bash script
  - ○ Benefit – submit & forget about it

- **Interactive job**
  - Run interactive session on the compute nodes
  - Benefit – exploratory work, troubleshooting etc.

# Batch jobs – a special bash script

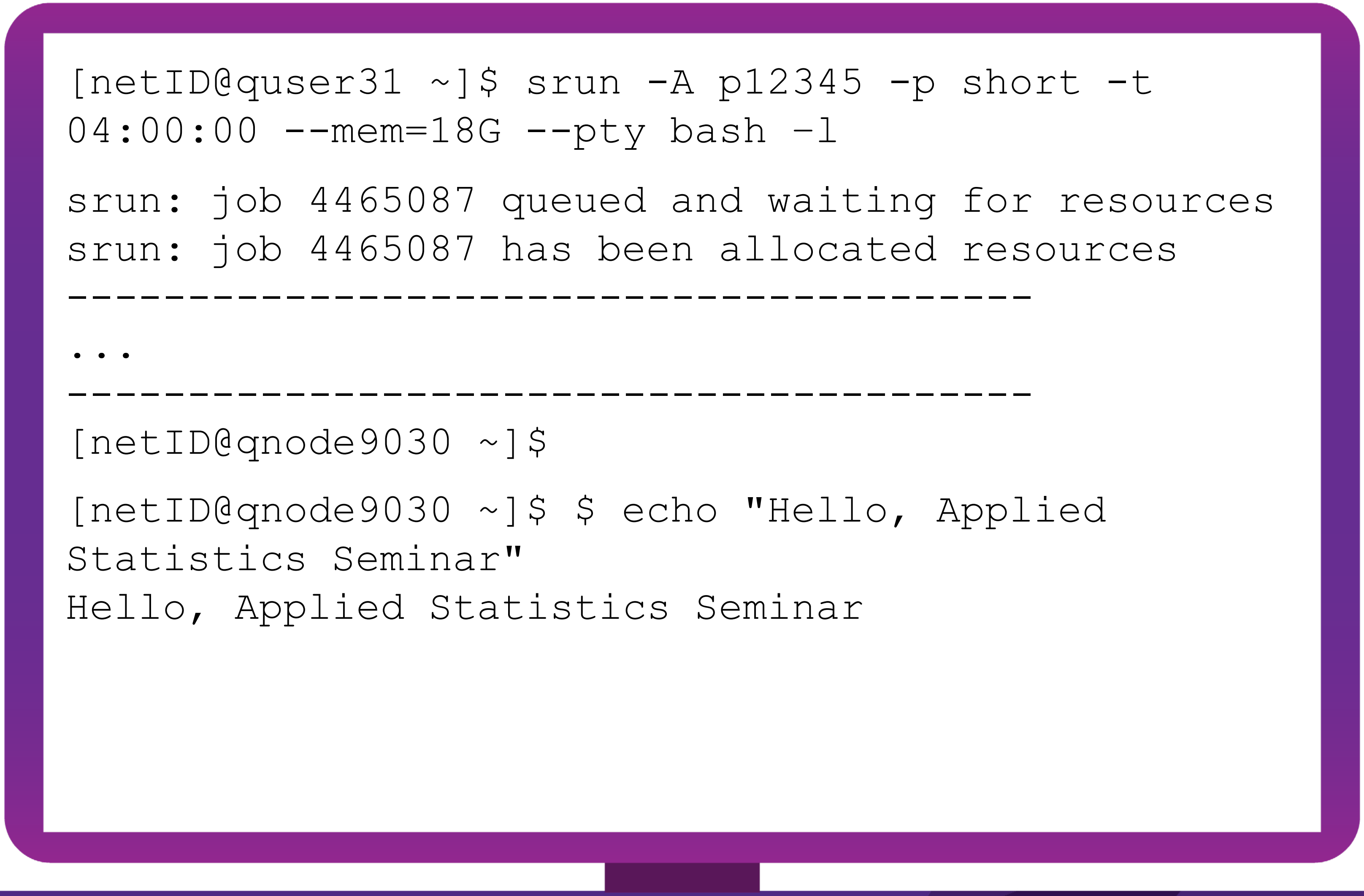
```
#!/bin/bash
#SBATCH --account=p12345
#SBATCH --partition=short
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --time=00:10:00
#SBATCH --mem-per-cpu=1G
#SBATCH --job-name=sample_job
#SBATCH --output=outlog
#SBATCH --mail-type=END,FAIL
#SBATCH --mail-user=email@northwestern.edu

module purge all
module load python/3.10.1

python hello_world.py
```

Requesting resources from SLURM

Code you want to run on Quest

Learn more about batch jobs!

# Interactive jobs

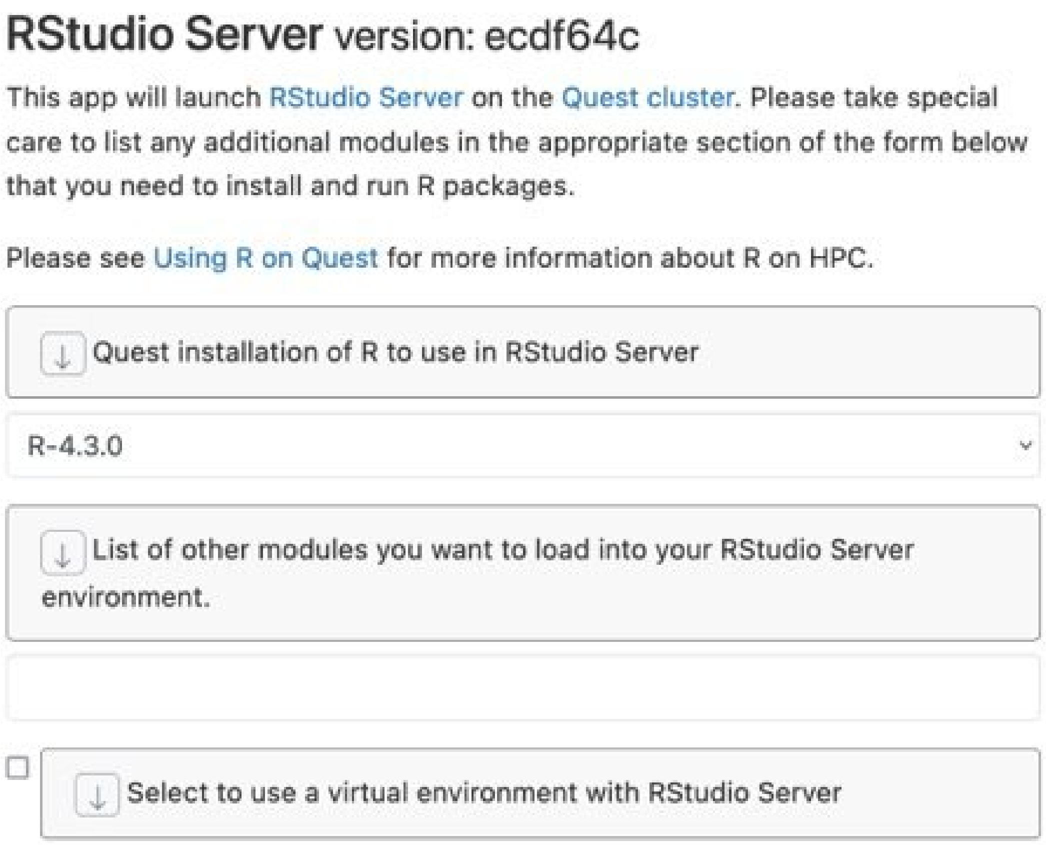


```
[netID@quser31 ~]$ srun -A p12345 -p short -t
04:00:00 --mem=18G --pty bash -l

srun: job 4465087 queued and waiting for resources
srun: job 4465087 has been allocated resources
----------------------------------------
...
----------------------------------------
[netID@qnode9030 ~]$

[netID@qnode9030 ~]$ $ echo "Hello, Applied
Statistics Seminar"
Hello, Applied Statistics Seminar
```

Learn more about interactive jobs!

# New service coming soon: Quest OnDemand!

- Browser-based tool
- Launch a variety of GUIs on a compute node without having to know how to use Slurm or the command line!
- Jupyter, RStudio, MATLAB, and more!
- Requires GlobalProtect VPN if you are off-campus



RStudio Server version: ecdf64c

This app will launch RStudio Server on the Quest cluster. Please take special care to list any additional modules in the appropriate section of the form below that you need to install and run R packages.

Please see Using R on Quest for more information about R on HPC.

Quest installation of R to use in RStudio Server

R-4.3.0

List of other modules you want to load into your RStudio Server environment.

□ Select to use a virtual environment with RStudio Server

# Live demonstration

# Questions?

**quest-help@northwestern.edu**

**Schedule a Zoom consultation with us** →

**In-person office hours:**
Mondays 3-4pm at the Mudd Library GIS Lab
(2nd Floor across from the bridge to Tech)

# EXTRA SLIDES: Special types of jobs and extra Slurm information

# Job Arrays

# Getting Started: Multicore

```
#!/bin/bash
#SBATCH --account=w10001  ## YOUR ACCOUNT pXXXX or bXXXX
#SBATCH --partition=w10001  ### PARTITION (buyin, short, normal, etc)
#SBATCH --nodes=1 ## how many computers do you need
#SBATCH --ntasks-per-node=4 ## how many cpus or processors do you need on each computer
#SBATCH --time=00:10:00 ## how long does this need to run
#SBATCH --mem-per-cpu=1G ## how much RAM do you need per CPU (affects your FairShare score!)
#SBATCH --job-name=sample_job  ## When you run squeue -u NETID this is how you can identify the job
#SBATCH --output=outlog ## standard out and standard error goes to this file
#SBATCH --mail-type=ALL ## you can receive e-mail alerts from SLURM when your job begins and when your job
finishes (completed, failed, etc)
#SBATCH --mail-user=email@u.northwestern.edu ## your email

module purge all
module load python-anaconda3
source activate /projects/intro/envs/slurm-py37-test

python slurm_test.py --nproc ${SLURM_NPROCS}
```

# Getting Started: Multimode/MPI

```
#!/bin/bash
#SBATCH --account=w10001  ## YOUR ACCOUNT pXXXX or bXXXX
#SBATCH --partition=w10001  ### PARTITION (buyin, short, normal, etc)
#SBATCH --nodes=2 ## how many computers do you need
#SBATCH --ntasks-per-node=4 ## how many cpus or processors do you need on each computer
#SBATCH --time=00:10:00 ## how long does this need to run
#SBATCH --mem-per-cpu=1G ## how much RAM do you need per CPU (this affects your FairShare score)
#SBATCH --job-name=sample_job  ## When you run squeue -u NETID this is how you can identify the job
#SBATCH --output=outlog ## standard out and standard error goes to this file
#SBATCH --mail-type=ALL ## e-mail alerts from SLURM about job status
#SBATCH --mail-user=email@u.northwestern.edu ## your email
#SBATCH --constraint="[quest7|quest8|quest9|quest10]" ### you want computers you have requested to be from either quest7 or quest8 or quest 9 or quest10 nodes, not a combination of nodes. Important for MPI

module purge all
module load python-anaconda3
source activate /projects/intro/envs/slurm-py37-test


mpiexec -n ${SLURM_NTASKS} python -m mpi4py.bench helloworld
```

# SLURM: Job-Array Example

```
#SBATCH --account=w10001  ## YOUR ACCOUNT pXXXX or bXXXX
#SBATCH --partition=w10001  ### PARTITION (buyin, short, normal, etc)
#SBATCH --array=0-9 ## number of jobs to run "in parallel"
#SBATCH --nodes=1 ## how many computers do you need
#SBATCH --ntasks-per-node=1 ## how many cpus or processors do you need on each computer
#SBATCH --time=00:10:00 ## how long does this need to run (remember different partitions have restrictions on this param)
#SBATCH --mem-per-cpu=1G ## how much RAM do you need per CPU (this effects your FairShare score so be careful to not ask for more than you need))
#SBATCH --job-name="sample_job_\${SLURM_ARRAY_TASK_ID}" ## use the task id in the name of the job
#SBATCH --output=sample_job.%A_%a.out ## use the jobid (A) and the specific job index (a) to name your log file
#SBATCH --mail-type=ALL ## you can receive e-mail alerts from SLURM when your job begins and when your job finishes (completed, failed, etc)
#SBATCH --mail-user=email@u.northwestern.edu ## your email

module purge all
module load python-anaconda3
source activate /projects/intro/envs/slurm-py37-test

IFS=$'\n' read -d '' -r -a lines < list_of_files.txt

python slurm_test.py --job-id $SLURM_ARRAY_TASK_ID --filename ${lines[$SLURM_ARRAY_TASK_ID]}
```

# SLURM: Job-Array Example (cont)

```
#SBATCH --account=w10001  ## YOUR ACCOUNT pXXXX or bXXXX
#SBATCH --partition=w10001  ### PARTITION (buyin, short, normal, etc)
#SBATCH --array=0-9%2 ## number of jobs to run "in parallel” the %2 restricts so that only 2 jobs max can be
running simultaneously
#SBATCH --nodes=1 ## how many computers do you need
#SBATCH --ntasks-per-node=1 ## how many cpus or processors do you need on each computer
#SBATCH --time=00:10:00 ## how long does this need to run (remember different partitions have restrictions on this
param)
#SBATCH --mem-per-cpu=1G ## how much RAM do you need per CPU (this effects your FairShare score so be careful to
not ask for more than you need))
#SBATCH --job-name="sample_job_\${SLURM_ARRAY_TASK_ID}" ## use the task id in the name of the job
#SBATCH --output=sample_job.%A_%a.out ## use the jobid (A) and the specific job index (a) to name your log file
#SBATCH --mail-type=ALL ## you can receive e-mail alerts from SLURM when your job begins and when your job
finishes (completed, failed, etc)
#SBATCH --mail-user=email@u.northwestern.edu ## your email

module purge all
module load python-anaconda3
source activate /projects/intro/envs/slurm-py37-test

IFS=$'\n' read -d '' -r -a lines < list_of_files.txt

python slurm_test.py --job-id $SLURM_ARRAY_TASK_ID --filename ${lines[$SLURM_ARRAY_TASK_ID]}
```

# Dependent Jobs

# SLURM: Dependency Example

```
#!/bin/bash

jid0=($(sbatch --time=00:10:00 --account=w10001 --partition=w10001 --nodes=1 --ntasks-per-node=1
--mem=8G --job-name=example --output=job_%A.out example_submit.sh))

echo "jid0 ${jid0[-1]}" >> slurm_ids

jid1=($(sbatch --dependency=afterok:${jid0[-1]} --time=00:10:00 --account=w10001 --
partition=w10001 --nodes=1 --ntasks-per-node=1 --mem=8G --job-name=example --output=job_%A.out -
-export=DEPENDENTJOB=${jid0[-1]} example_submit.sh))

echo "jid1 ${jid1[-1]}" >> slurm_ids

jid2=($(sbatch --dependency=afterok:${jid1[-1]} --time=00:10:00 --account=w10001 --
partition=w10001 --nodes=1 --ntasks-per-node=1 --mem=8G --job-name=example --output=job_%A.out -
-export=DEPENDENTJOB=${jid1[-1]} example_submit.sh))

echo "jid2 ${jid2[-1]}" >> slurm_ids
```

# SLURM: Dependency Example

```
#!/bin/bash
#SBATCH --mail-type=ALL ## you can receive e-mail alerts from SLURM when your job begins and
when your job finishes (completed, failed, etc)
#SBATCH --mail-user=email@u.northwestern.edu ## your email


if [[ -z "${DEPENDENTJOB}" ]]; then
    echo "First job in workflow"
else
    echo "Job started after " $DEPENDENTJOB
fi


module purge all
module load python-anaconda3
source activate /projects/intro/envs/slurm-py37-test


python --version
python slurm_test.py
```

# Architecture Constraints

# SLURM: Constraints Example

```
#!/bin/bash
#SBATCH --account=w10001  ## YOUR ACCOUNT pXXXX or bXXXX
#SBATCH --partition=w10001  ### PARTITION (buyin, short, normal, etc)
#SBATCH --nodes=2 ## how many computers do you need
#SBATCH --ntasks-per-node=4 ## how many cpus or processors do you need on each computer
#SBATCH --time=00:10:00 ## how long does this need to run (remember different partitions have restrictions on this
param)
#SBATCH --mem-per-cpu=1G ## how much RAM do you need per CPU (this effects your FairShare score so be careful to
not ask for more than you need))
#SBATCH --job-name=sample_job  ## When you run squeue -u NETID this is how you can identify the job
#SBATCH --output=outlog ## standard out and standard error goes to this file
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finishes (completed, failed, etc)
#SBATCH --mail-user=email@u.northwestern.edu ## your email
#SBATCH --constraint="[quest7|quest8|quest9|quest10]" ### you want computers you have requested to
be from either quest7 or quest8 or quest9 or quest10 nodes, not a combination of nodes. Useful for
MPI applications.

module purge all
module load python-anaconda3
source activate /projects/intro/envs/slurm-py37-test


mpiexec -n ${SLURM_NTASKS} python -m mpi4py.bench helloworld
```

# SLURM Environmental Variables

# SLURM: Environmental Variables

```
[quser21 ~]$ srun -N 2 --ntasks-per-node=5 --mem=10G --account=a9009 --partition=all
--time=00:10:00 --pty bash -l
…
…
[qnode0156 ~]$ printenv | grep SLURM
SLURM_NODELIST=qnode[0156-0157]
SLURM_NTASKS_PER_NODE=5
SLURM_NNODES=2
SLURM_JOBID=8177560
SLURM_NTASKS=10
SLURM_SUBMIT_DIR=/home/tempuser03
SLURM_NPROCS=10
```