Introduction to Quest

Please set up your screen to have Zoom on one half of the screen and a terminal or web browser on the other half.

Janna Nugent, Sr. Computational Biology Specialist
NUIT Research Computing

Northwestern
INFORMATION TECHNOLOGY

Please set up your screen to have Zoom on one half of the screen and a terminal or web browser on the other half.

How this workshop will work

- Interactive sections mixed with slides
- Slides will be available after the workshop
- Please ask questions in the chat or “Raise Hand” for help (button under “Participants”)
- Two 5 minute breaks
- This workshop is being recorded

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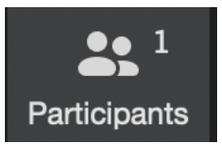
“Raise Hand” if you don’t have a Quest account

Click here →



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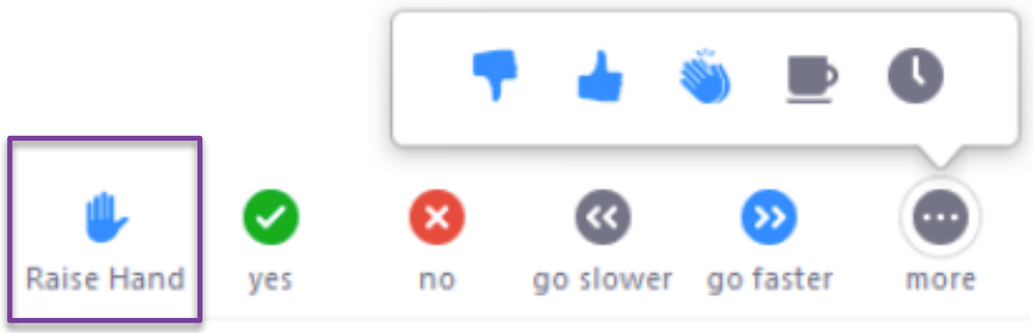

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Learn About

- Research Computing
- Quest System Architecture
- Research Allocations on Quest
- Parallel Computing
- File Sharing
- Getting Started:logging in, batch & interactive job submission

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Research Computing: the Consultants

We are a team under Northwestern Information Technology with research backgrounds in:

Social Sciences
Computer Science
Materials Science
Engineering
Astrophysics
Data Science
Bioinformatics
Cloud Computing
Data Workflow
Data Management
Visualizations

quest-help@northwestern.edu

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Alper Kinaci

Janna Nugent

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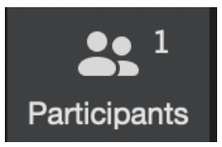

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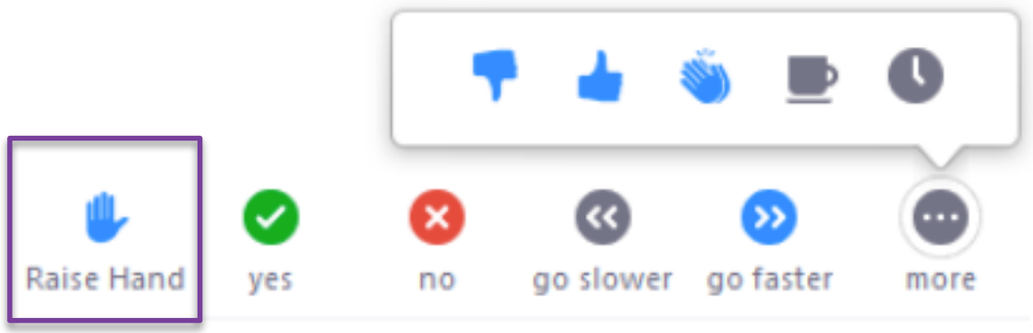

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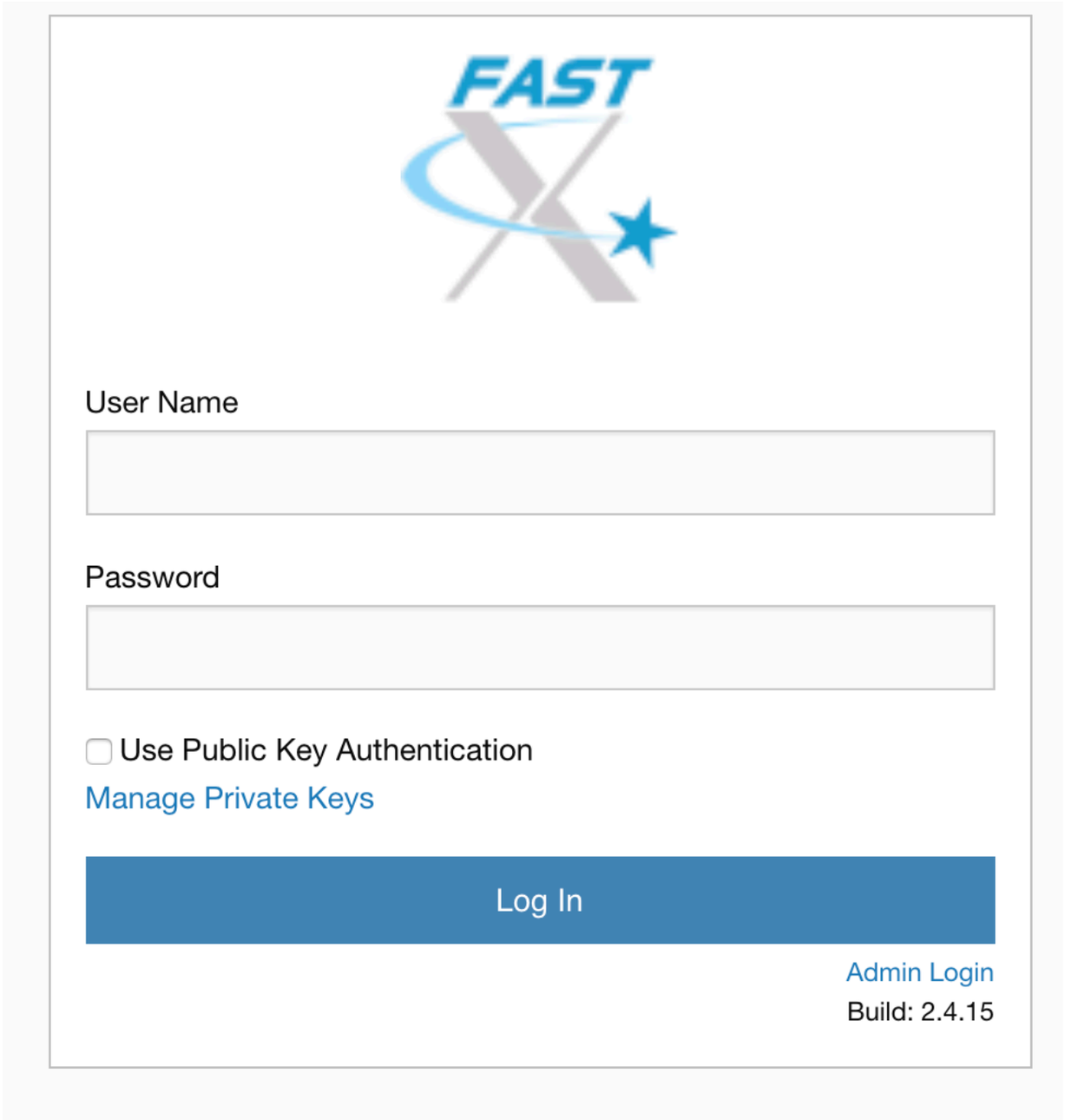
Login to Quest

Make sure you're connected to Northwestern's VPN

From browser: http://quest.northwestern.edu:3000

Login to Quest

http://quest.northwestern.edu:3000



If you don't see this, check you're on the VPN

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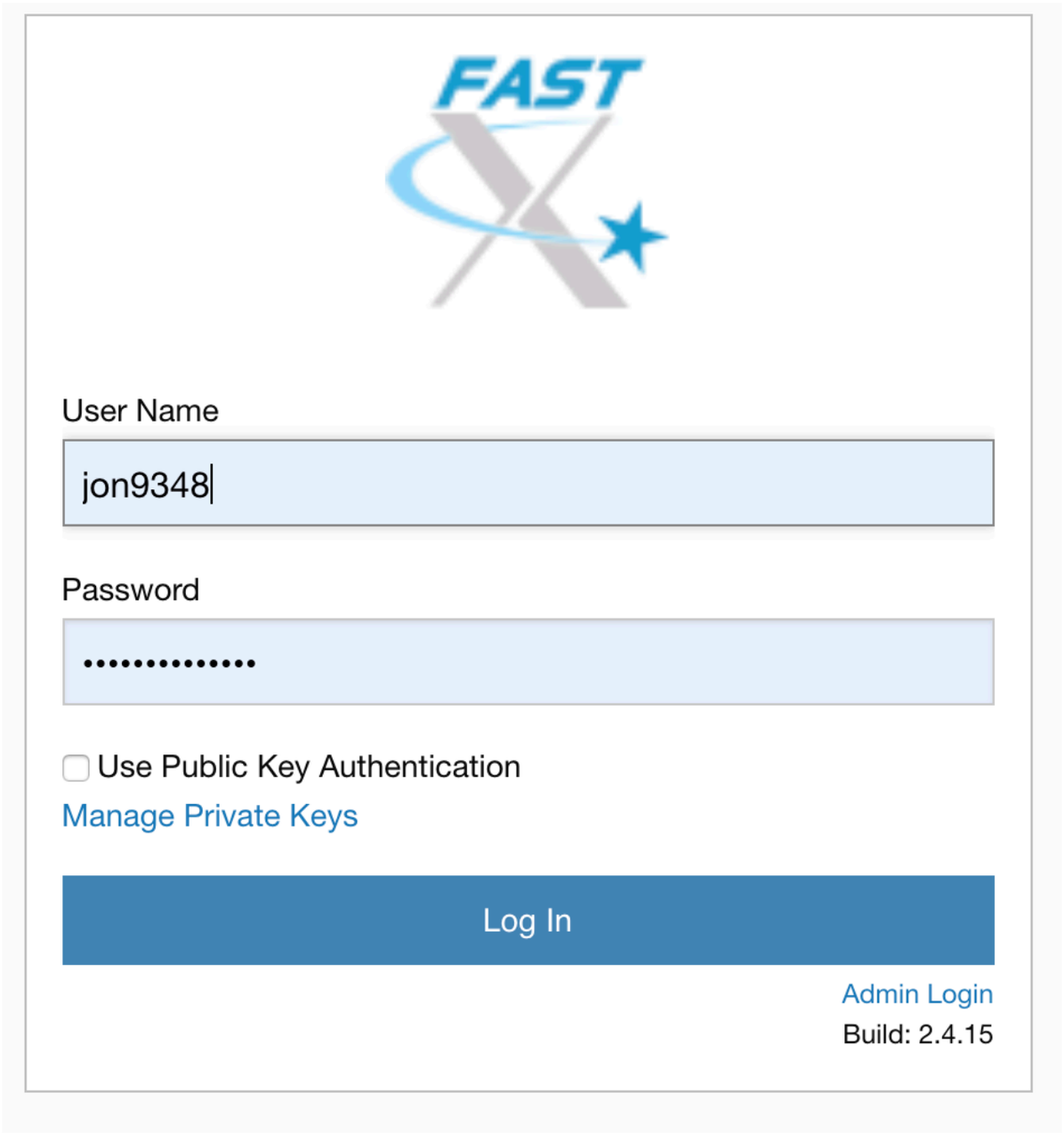
http://quest.northwestern.edu:3000



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Login to Quest

http://quest.northwestern.edu:3000

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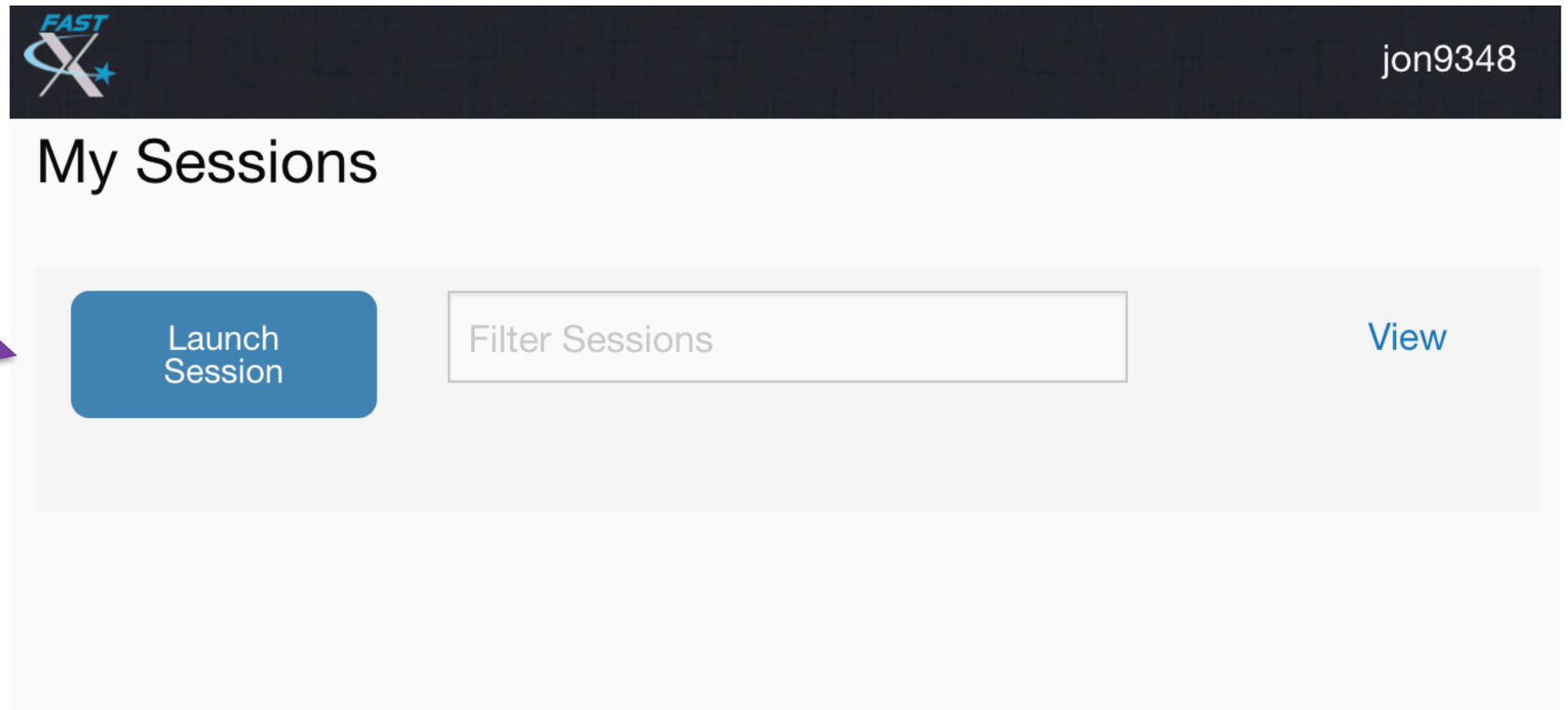
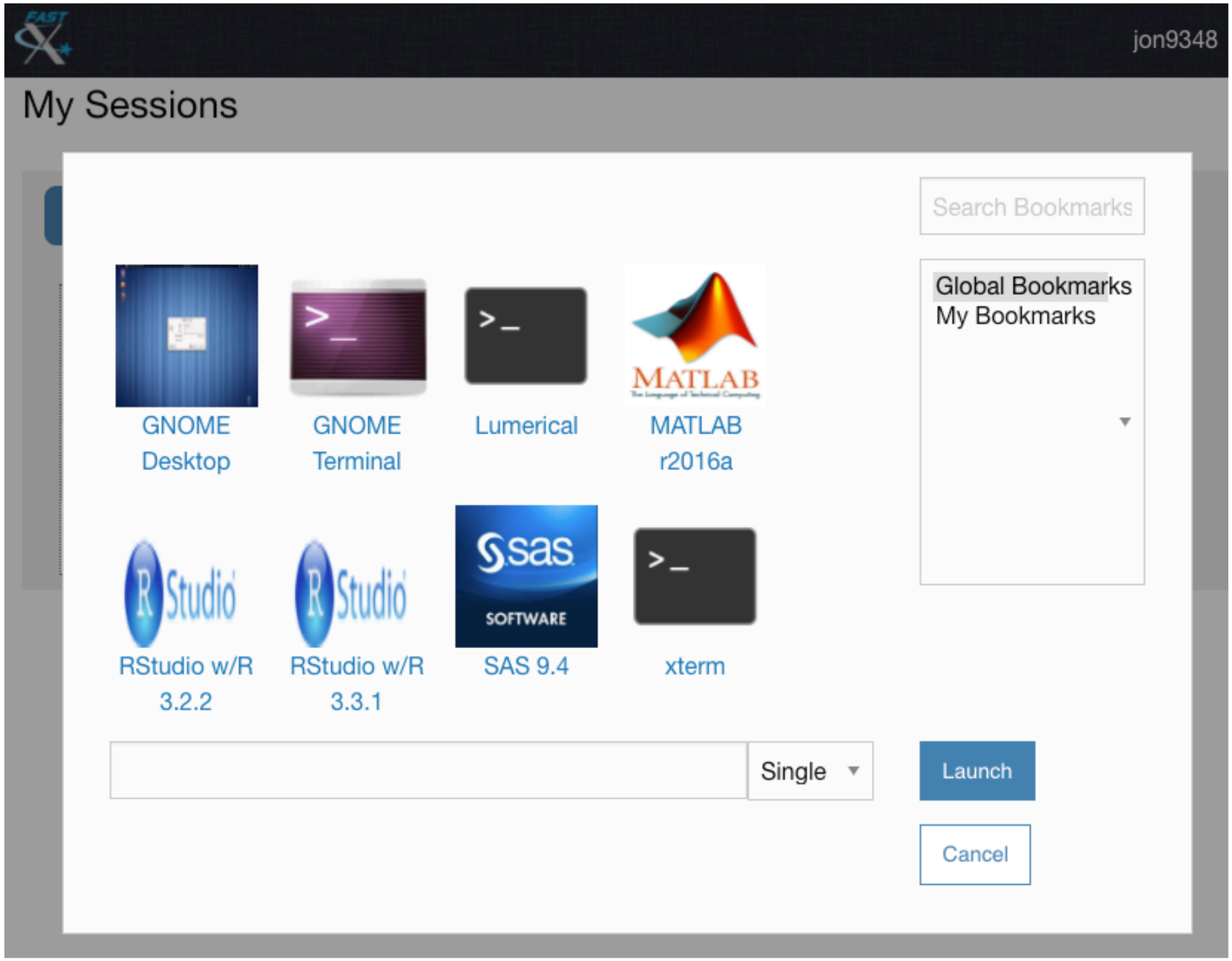


Click the “Launch Session” button

Login to Quest

http://quest.northwestern.edu:3000



Login to Quest

http://quest.northwestern.edu:3000

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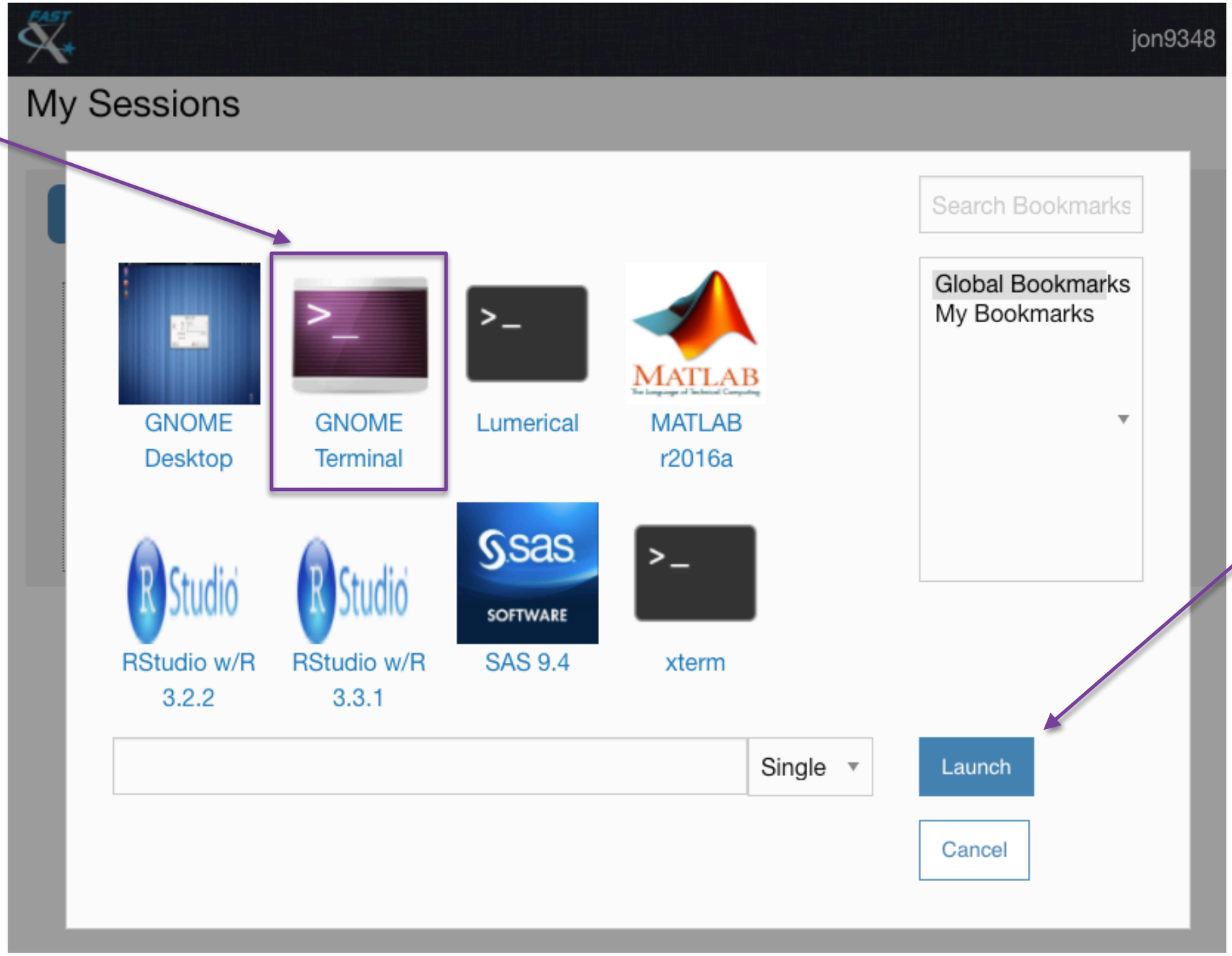
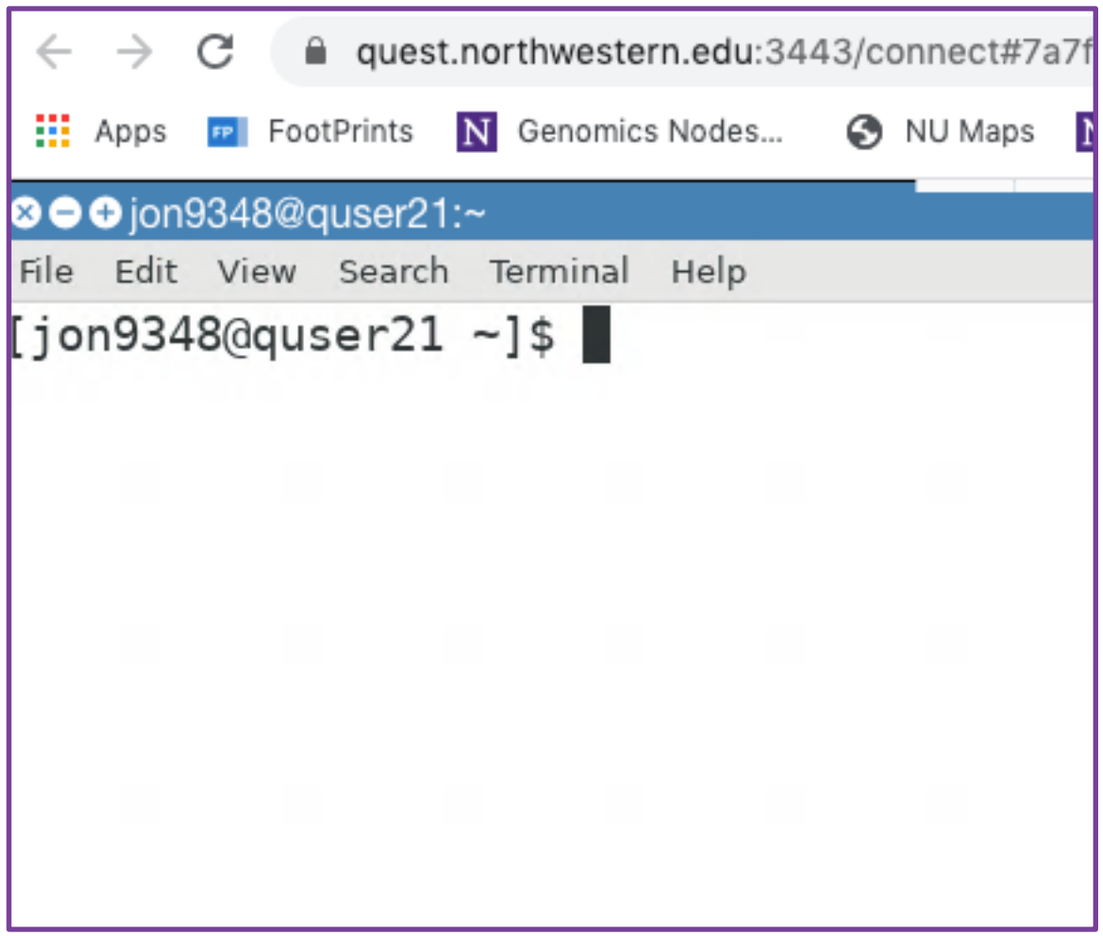


2) Click

Login to Quest

http://quest.northwestern.edu:3000



Success!

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“Raise Hand” if you can’t login

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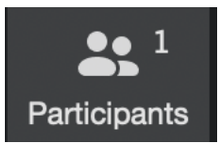

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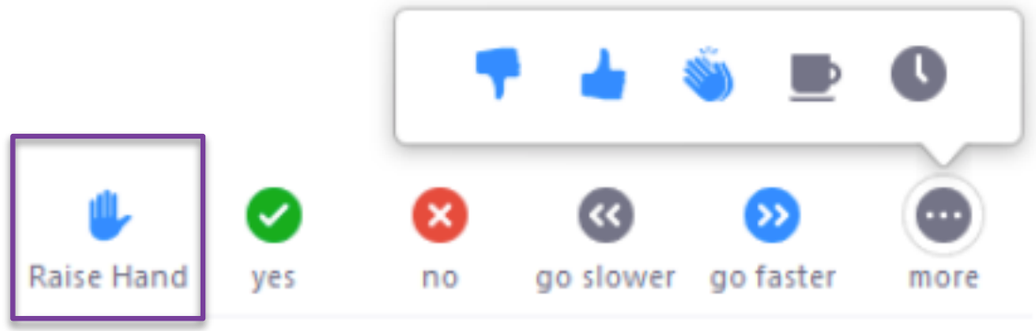

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[jon9348@quser22 ~]$
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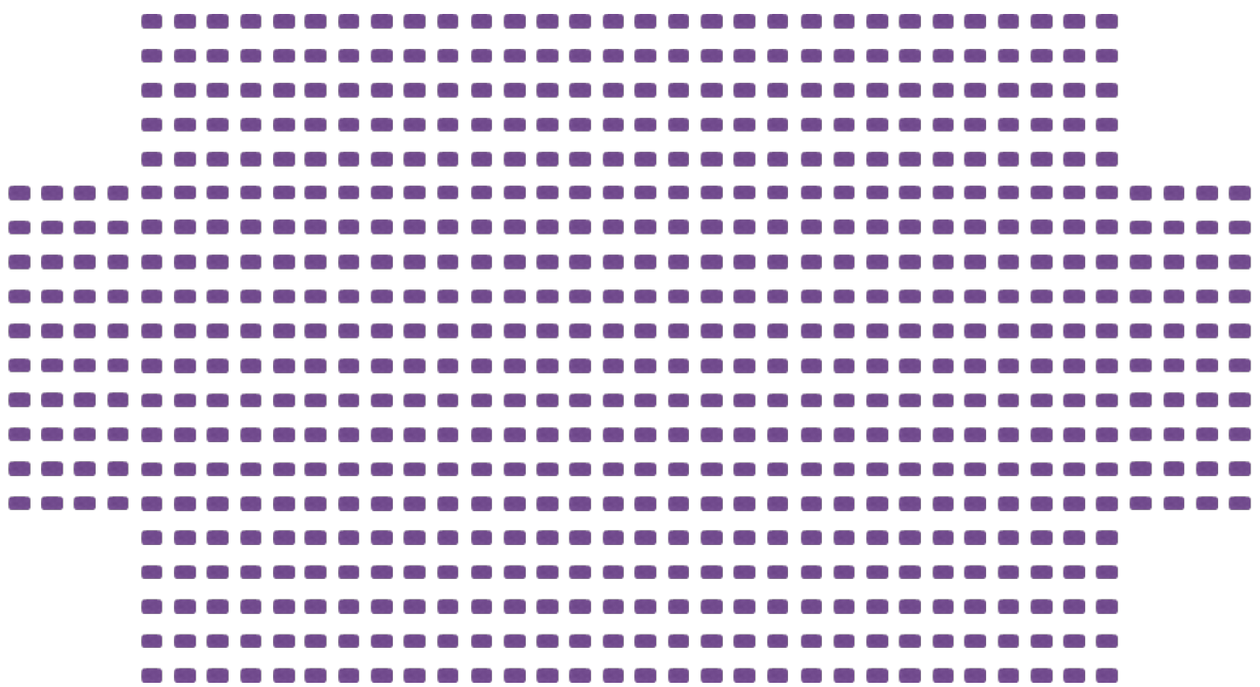
high-performance compute cluster

high-performance compute cluster

750 computers



high-performance compute cluster

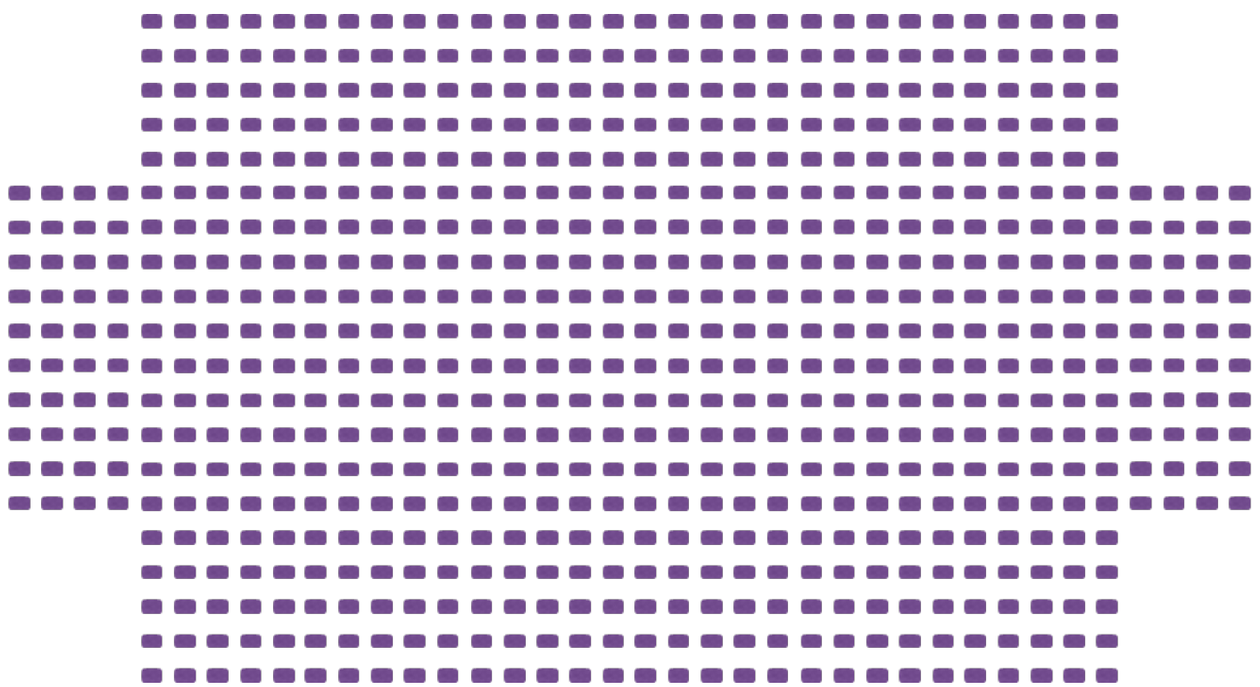
computer = “node”

nodes in racks

high-performance compute cluster

high-performance compute cluster

750 nodes



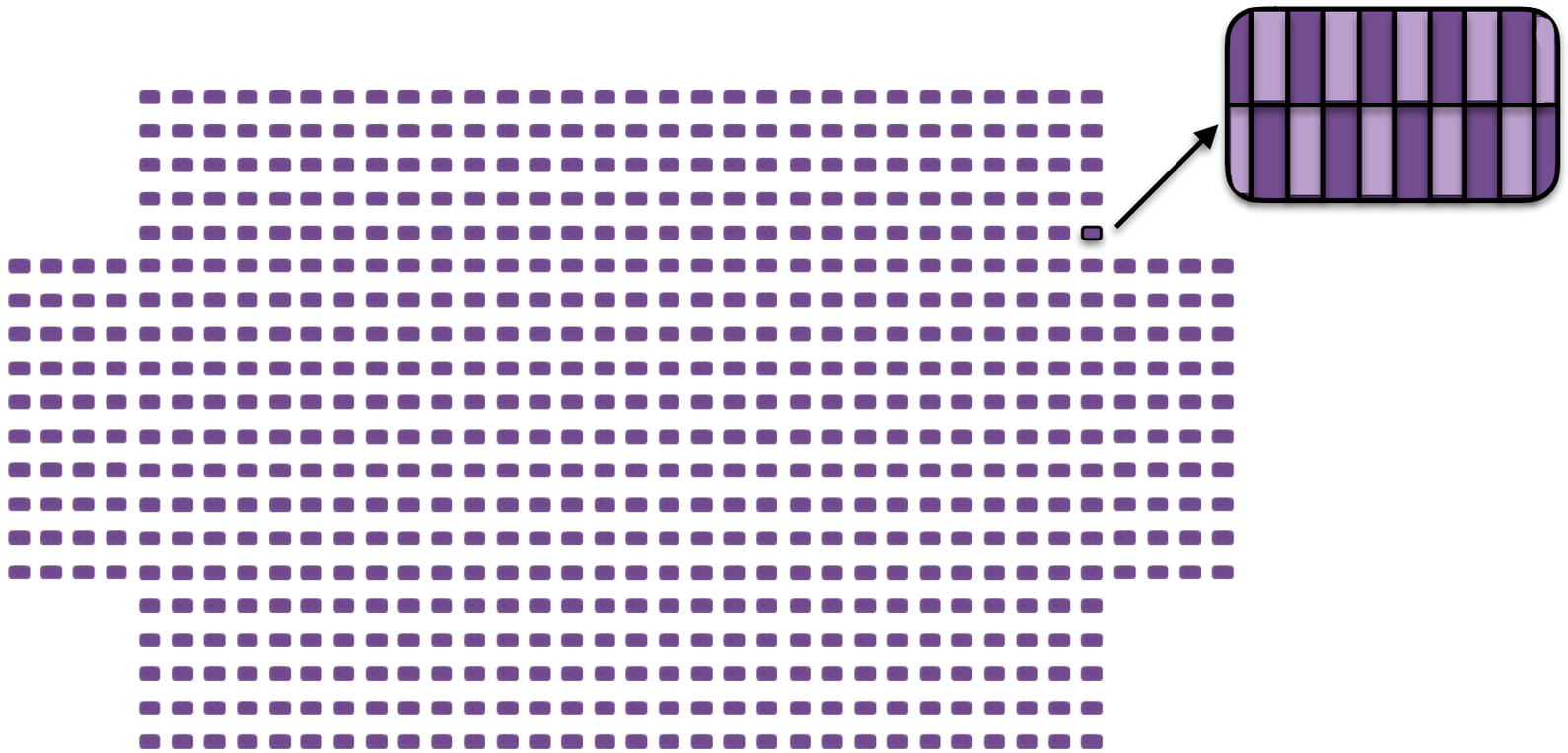
high-performance compute cluster

	1	750
	Desktop Computer	**Quest Node**
Processor Speed	2.2 MHz	2.5 - 3.3 MHz
Cores	2-4	24-40
Memory (RAM)	8 Gb	96-192 Gb

Quest has 25,000 cores

high-performance compute cluster

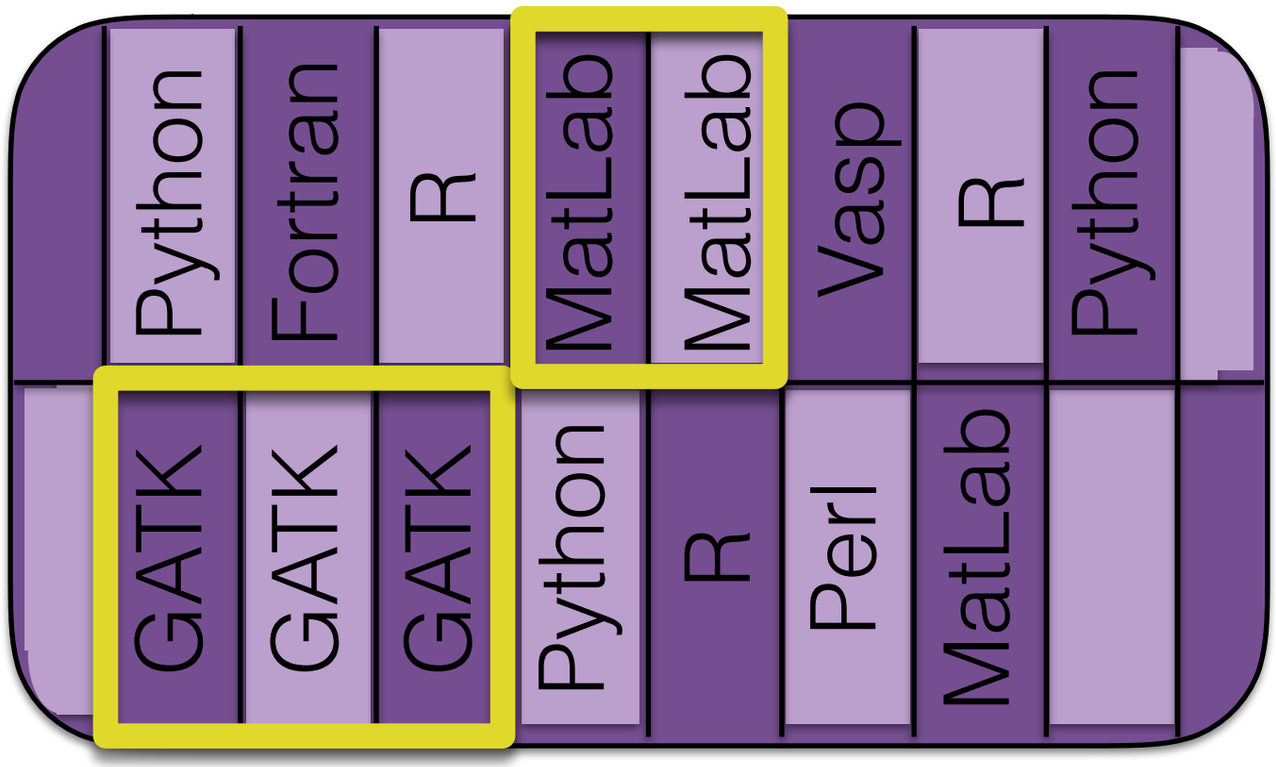
Each of the 750 nodes has 24-40 **cores**



Cores can also be called processors or CPUs
- they are what a thread or a task runs on

high-performance compute cluster

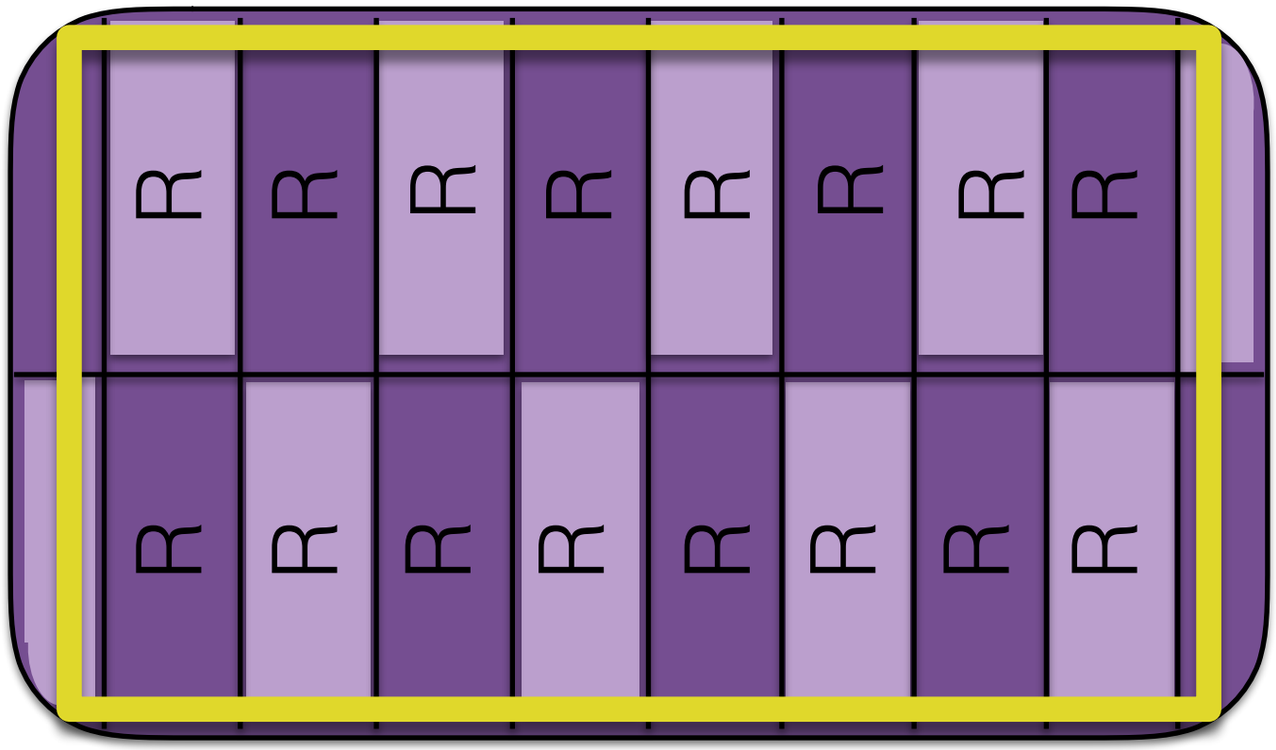
Each node can run **jobs** from
24-40 researchers at once



A job consists of a pre-packaged sequence of commands run on a node for a user

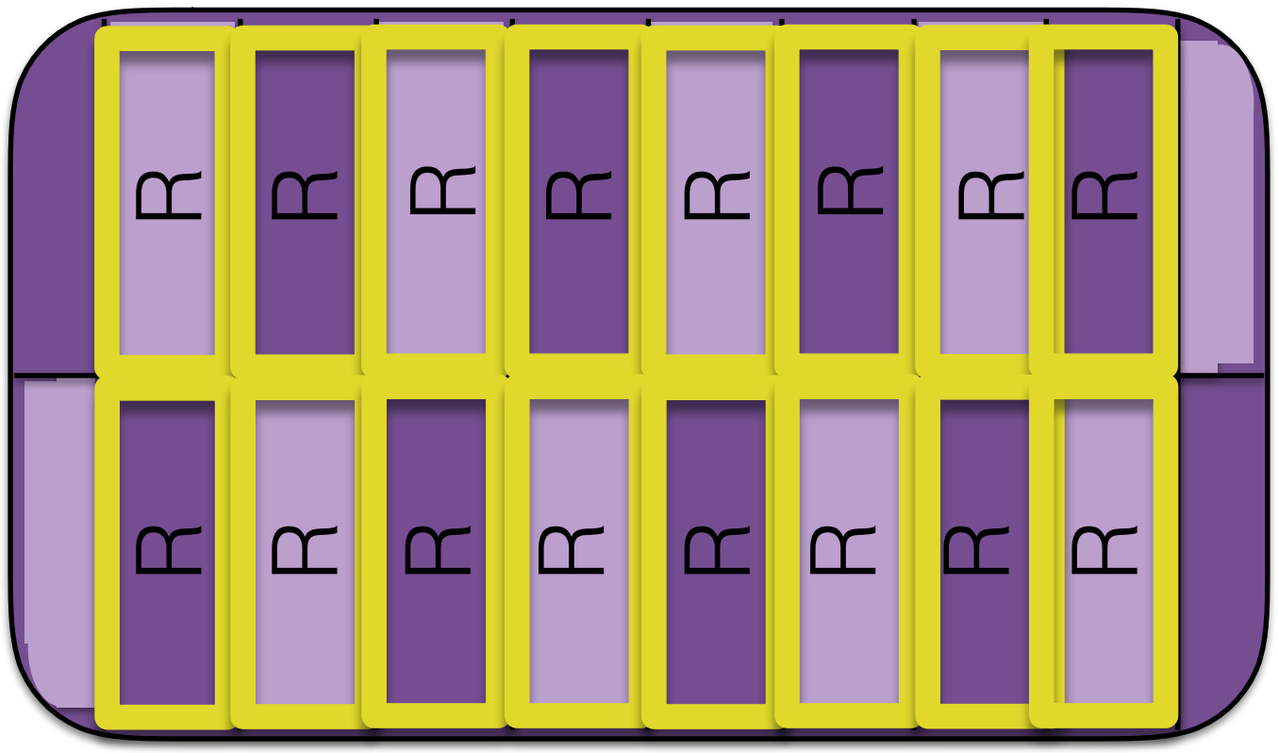
high-performance compute cluster

Each node can run jobs with 24-40 threads at once, using all of the cores and memory of the node



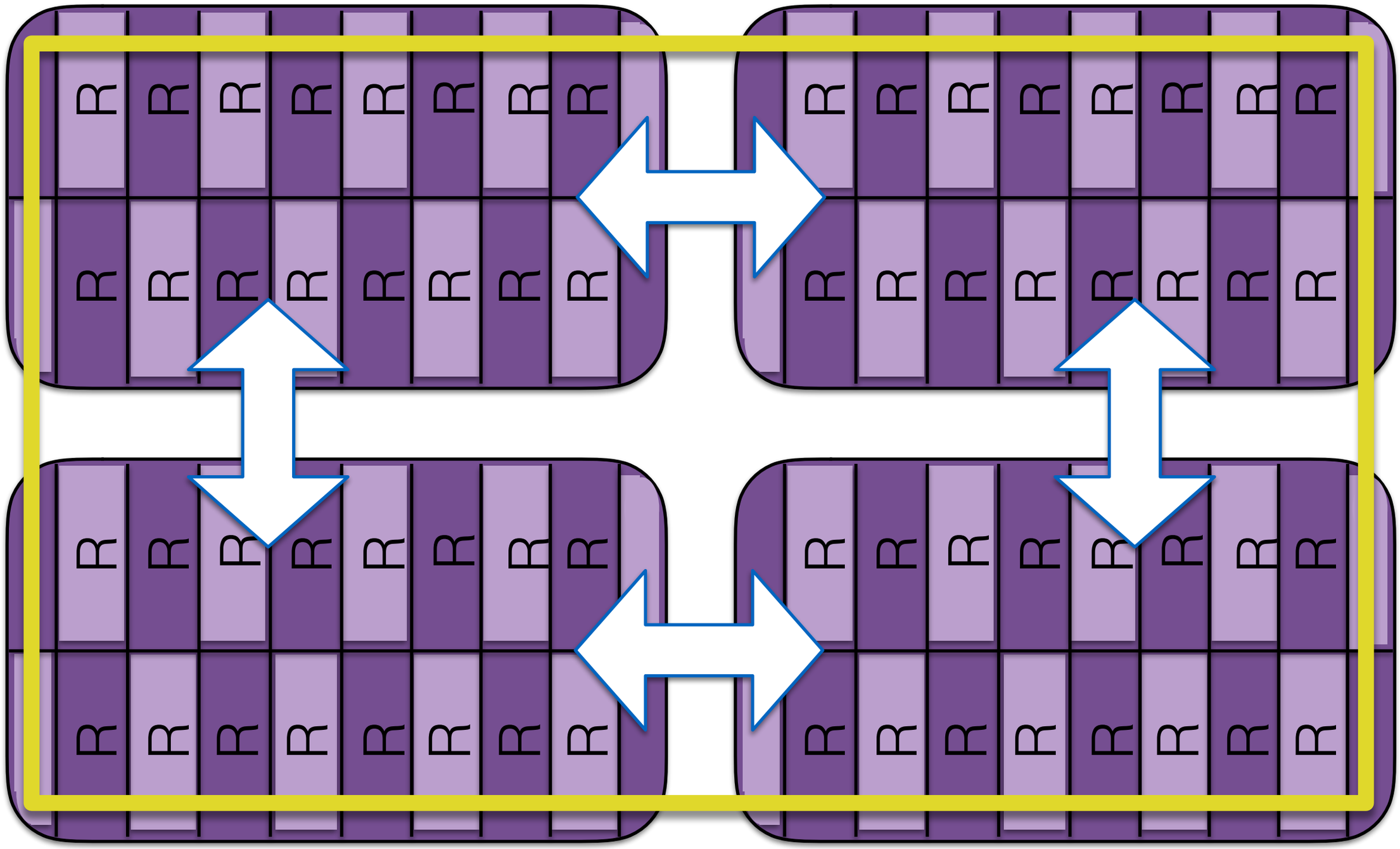
high-performance compute cluster

Each researcher can run thousands of jobs at once and can have up to 5,000 jobs waiting to run at any time



Multiple independent jobs parallel computing: High-throughput

high-performance compute cluster



1 job, multiple nodes parallel computing: OpenMP, MPI

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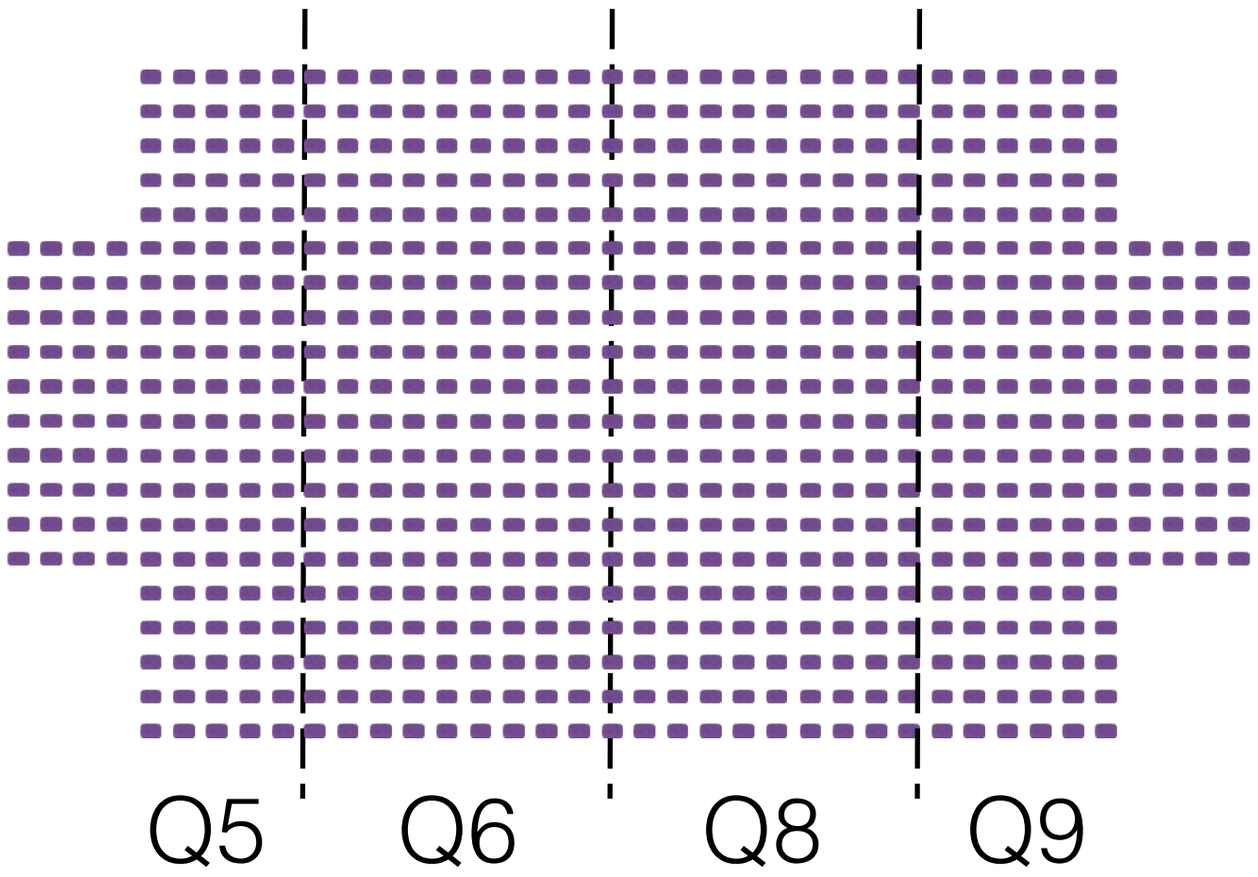
[jon9348@quser22 ~]$
```

high-performance compute cluster

Node Architectures: 4 Generation of Nodes



128 GB RAM (Q5, Q6)

96 GB RAM (Q8)

192 GB RAM (Q9)

Q5 → 24 cores/node
Q6 → 28 cores/node
Q8 → 28 cores/node
Q9 → 40 cores/node

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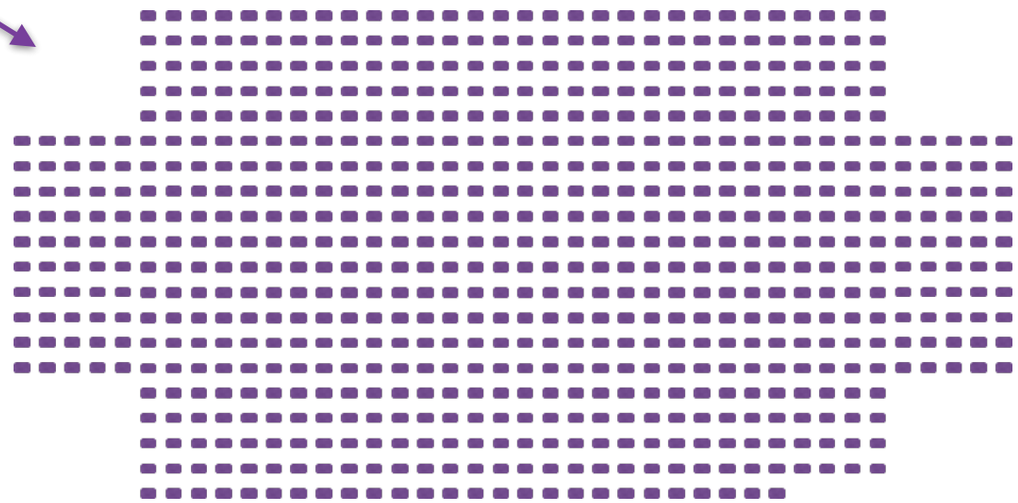
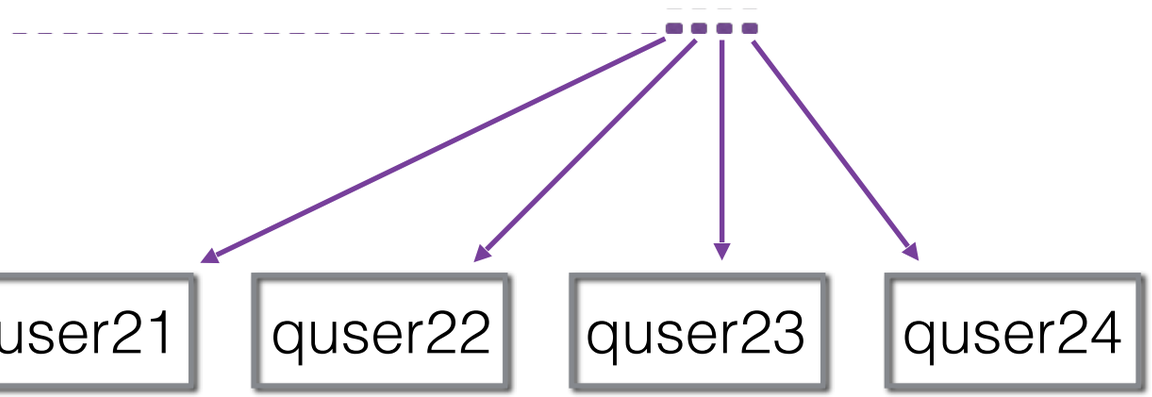
Quest: High Performance Compute Cluster

compute nodes





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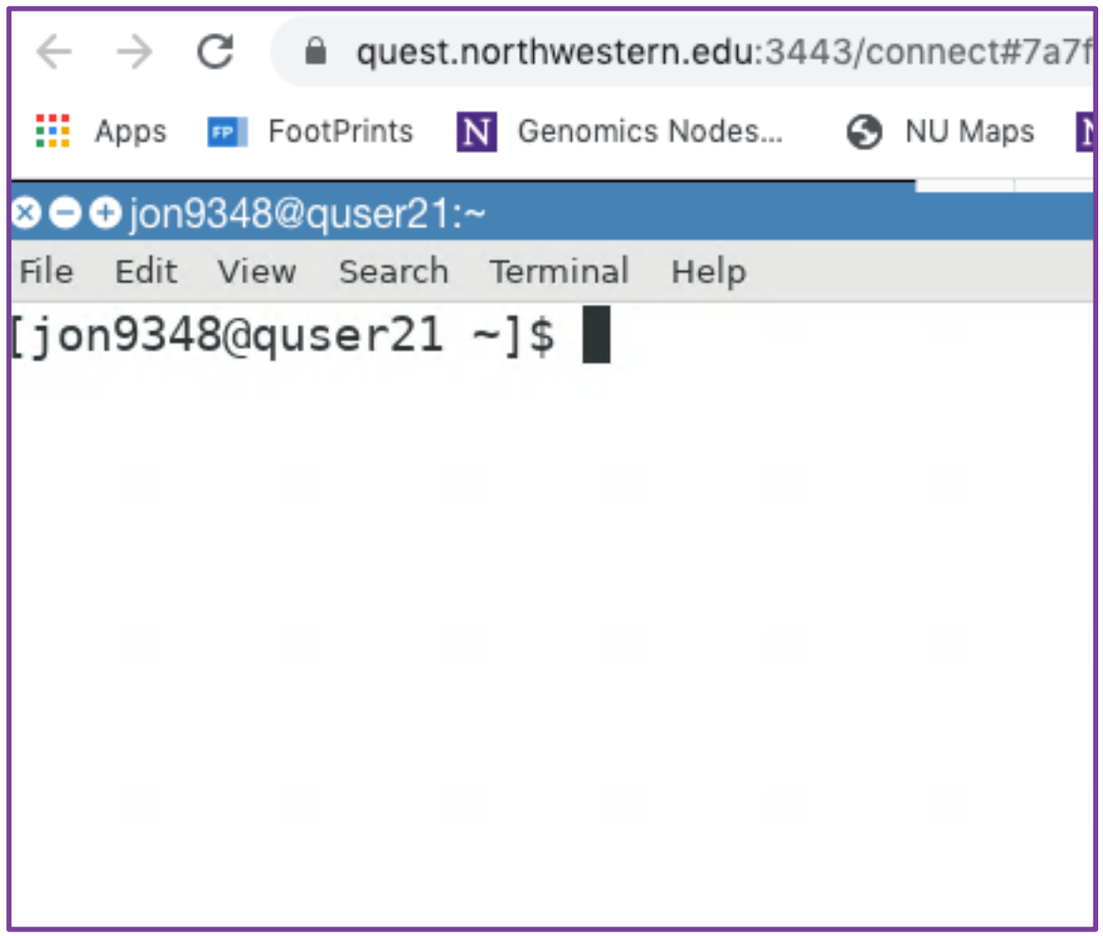
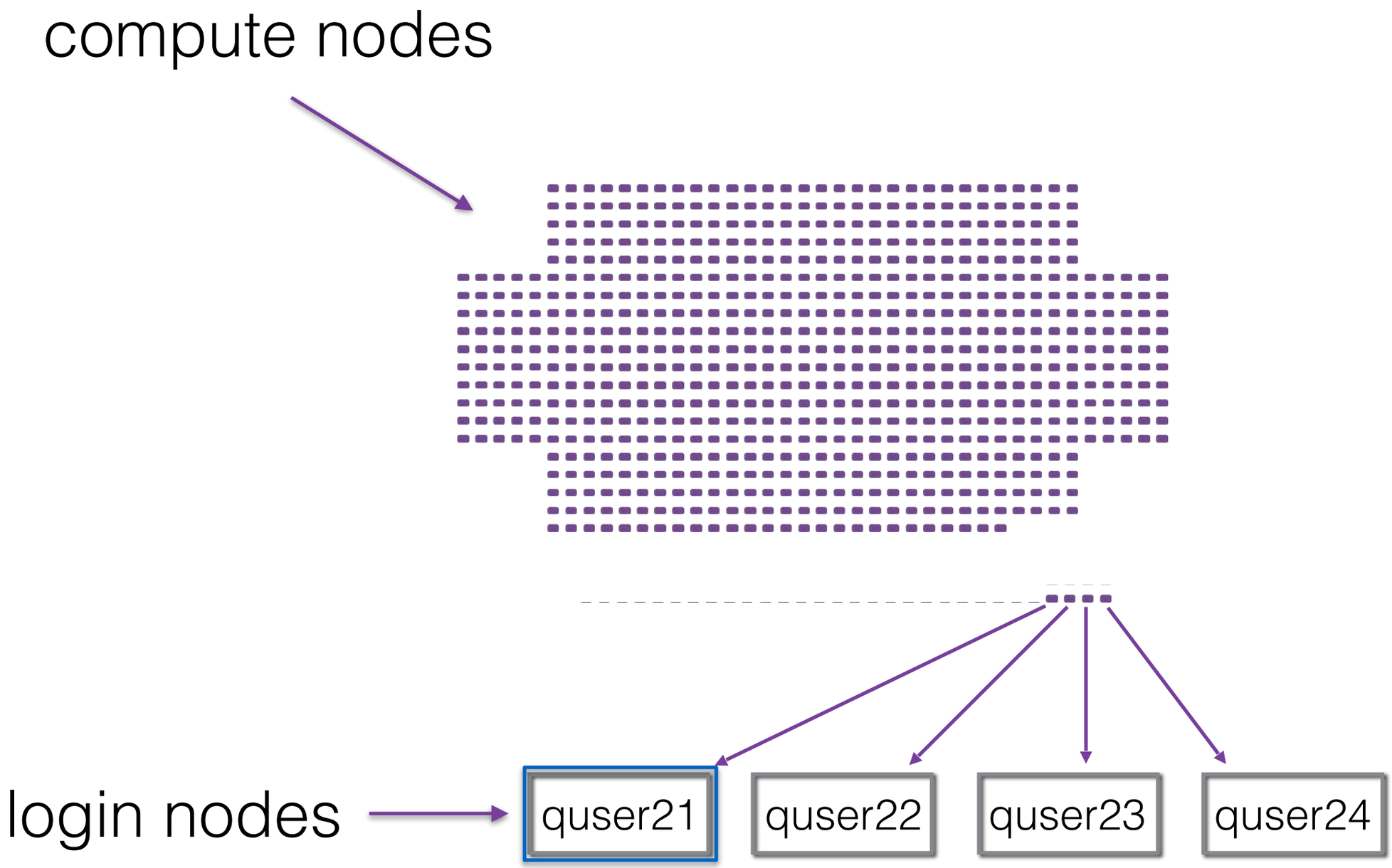


Success!

Quest: High Performance Compute Cluster



Interactive on Quest

BREAK

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##  \_____\_____\\______/  |_______|_______/       |__|       ##
##                                                            ##
##################################################################

Welcome to Quest high-performance compute cluster: enabling 10 years of computational research at Northwestern.

Quest has four node architectures, which you can specify in your script (for example: #SBATCH --constraint=quest6
).

Quest architectures and node specifications are below:
- quest5: 24 cores & 128 GB memory per node
- quest6: 28 cores & 128 GB memory per node
- quest8: 28 cores &  96 GB memory per node
- quest9: 40 cores & 192 GB memory per node

Users cannot request more than 4 cores and/or 4 GB of memory in total for all commands and code they are running
on a login node.

Please remember that Quest is not approved for contractually or legally restricted data. Ensure sensitive data is
 anonymized or de-identified before being moved to quest. Contact us if you need a computing environment for the
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Information on Quest can be found at http://www.it.northwestern.edu/research/user-services/quest/index.html.

Quest enforces memory limits on jobs. For more information, please see https://kb.northwestern.edu/specifying-mem
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Quest Storage and Data Policy is available at https://www.it.northwestern.edu/research/user-services/storage/stor
age-data-policy.html

If you have any other questions or would like to purchase nodes or storage for dedicated usage, please contact us
 at quest-help@northwestern.edu.
[jon9348@quser22 ~]$
```

Quest High Performance Computing Cluster

About Quest

- System Overview
- Technical Specifications
- Procedural Guidelines
- Citation/Acknowledgement of Use
- Rights and Responsibilities for the Use of Central Network and Computing Resources at Northwestern University
- Software

Allocations and Resources

- Types of Allocations and Application Submission Guidelines
- Apply, Renew, or Join an Allocation
- Purchasing Resources on Quest
- Quest Storage
- Genomics Compute Cluster on Quest
- Quest Analytics Nodes
- Quest Storage and Data Policy

Support

- Request a Consultation
- Logging in to Quest
- Quest Quick Start Guide
- Quest Documentation and Tutorials
- How-to Video Series
- quest-help@northwestern.edu

```
Last login: Wed Apr  8 17:04:24 2020 from vpn-165-124-161-6.vpn.northwestern.edu
##################################################################
##   ______      __    __   _______     _______.___________.  ##
##  /  __  \    |  |  |  | |   ____|   /       |           |  ##
## |  |  |  |   |  |  |  | |  |__     |   (----`---|  |----`  ##
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##################################################################

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```
Last login: Wed Apr  8 17:04:24 2020 from vpn-165-124-161-6.vpn.northwestern.edu
##################################################################
##   ______      __    __   _______     _______.___________.  ##
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##################################################################

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##   ______      __    __   _______     _______.___________.  ##
##  /  __  \    |  |  |  | |   ____|   /       |           |  ##
## |  |  |  |   |  |  |  | |  |__     |   (----`---|  |----`  ##
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##                                                            ##
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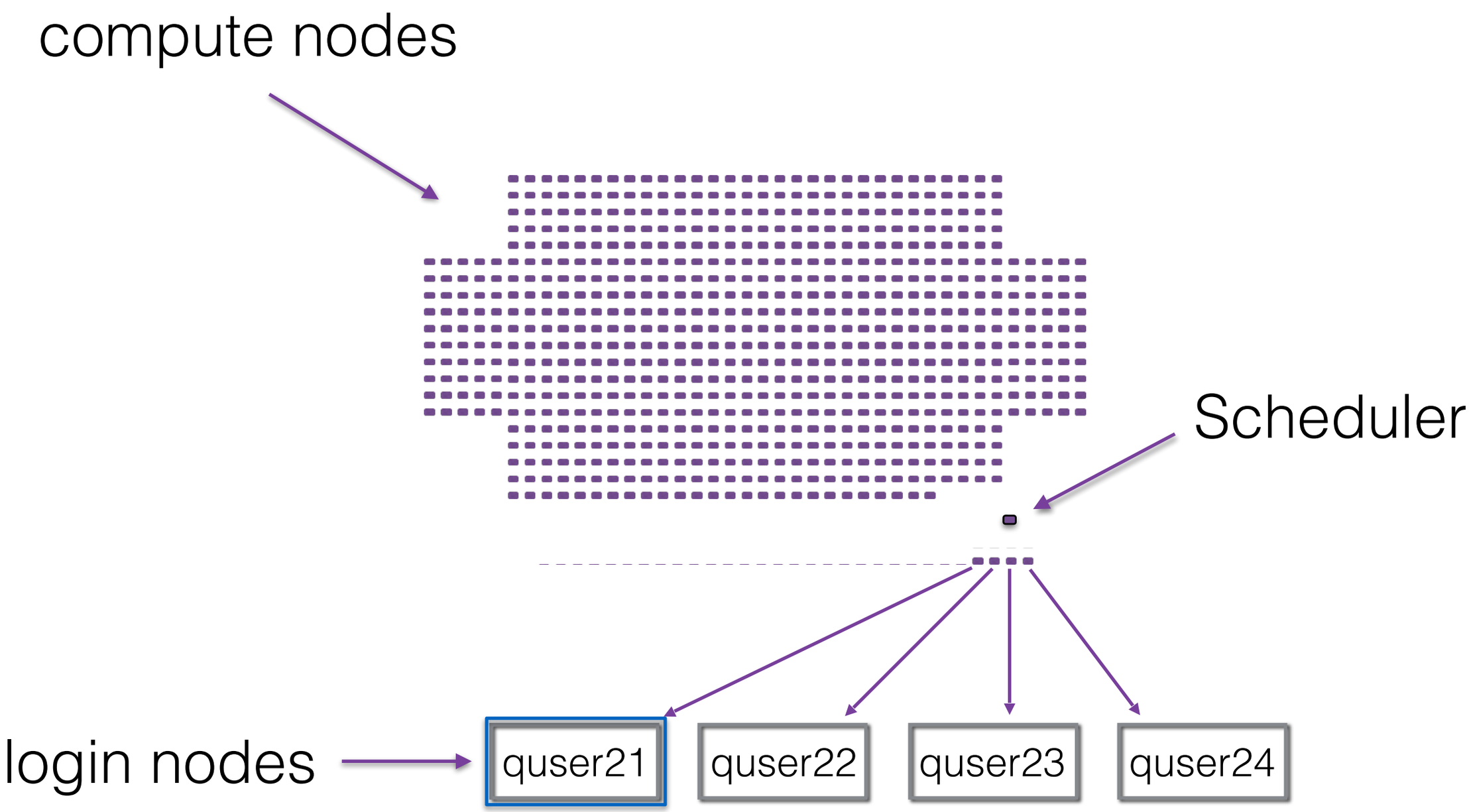
[jon9348@quser22 ~]$
```

Interactive on Quest

Quest: High Performance Compute Cluster



The Scheduler

login node

"sbatch submit.sh"

scheduler

```
#SBATCH -A
<allocationID>
#SBATCH -p <queue_type>
#SBATCH  -N 1
.
.
```

compute node

compute node

compute node

compute node

Account vs. Allocation

Account

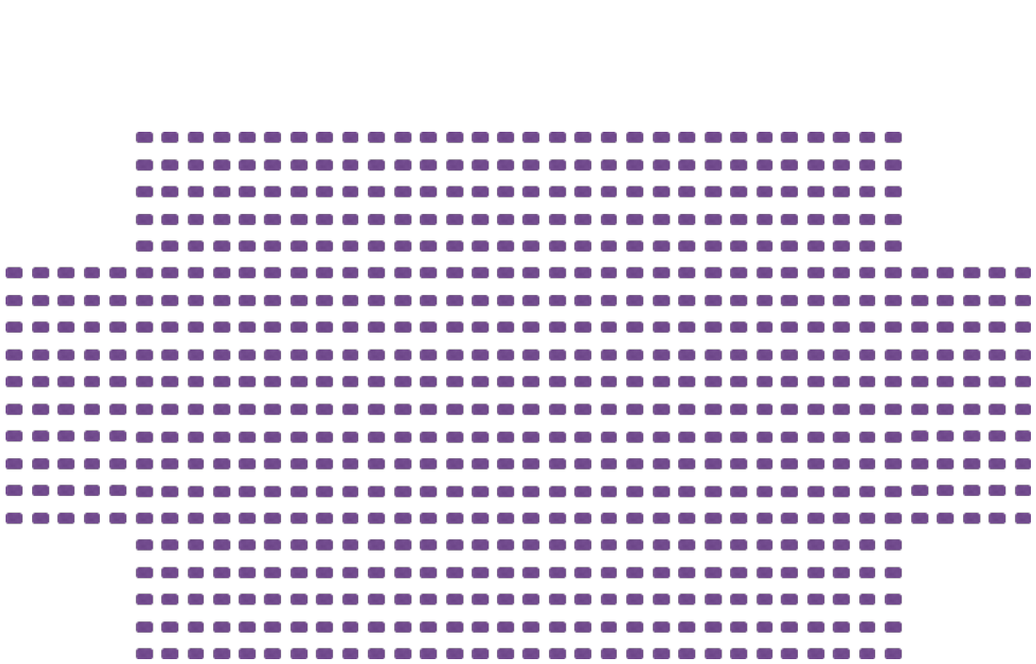
- Private
- /home/<netID>
- Backed up
- 80Gb storage quota

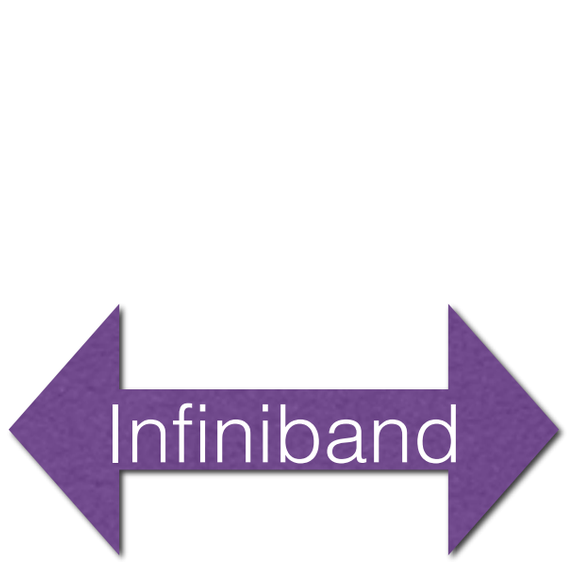
Allocation

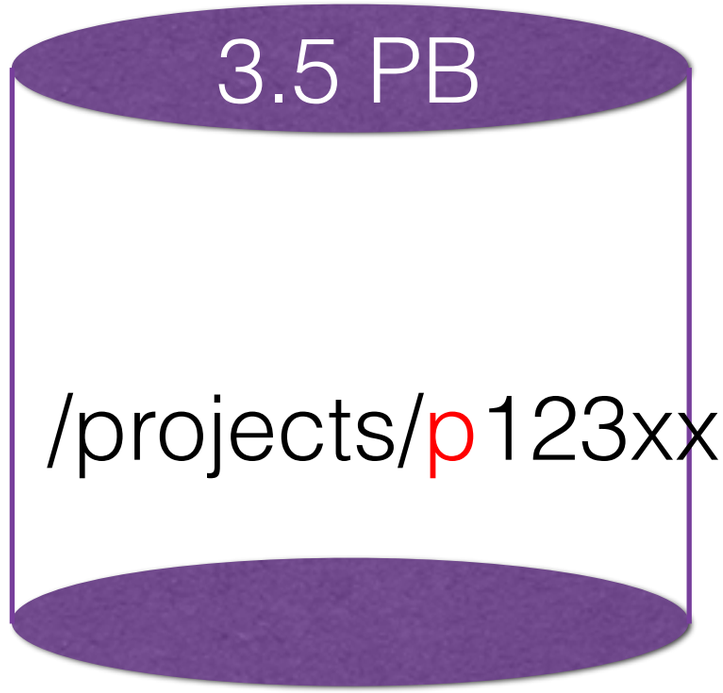
- Group
- Shared access to time on the compute nodes
- Shared storage: /projects/<allocation>
- Not backed up

Allocation Types: General Access

Research I Allocation, 500GB storage	computational need < 100K hour
Research II Allocation, 2TB storage	computational need > 100K hour
Classroom Allocation, 500GB storage	computational need < 100K hour



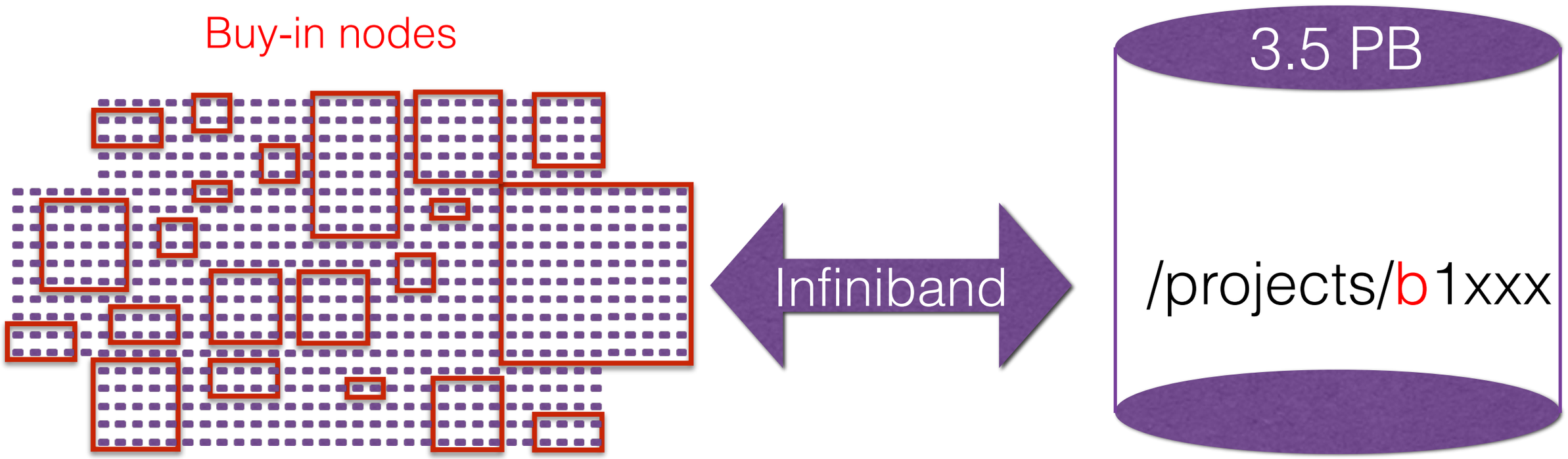




http://www.it.northwestern.edu/research/user-services/quest/allocation-guidelines.html

Allocation Types: Buy-in

Full access to compute nodes & persistent storage for 5 years



http://www.it.northwestern.edu/research/user-services/quest/full-access.html

Genomics Compute Cluster

- Allocation b1042
- Dedicated to genomics research
- Free to all genomics researchers at Northwestern
- 2,600 cores
- Dedicated high-memory nodes
- 175 Tb of scratch space

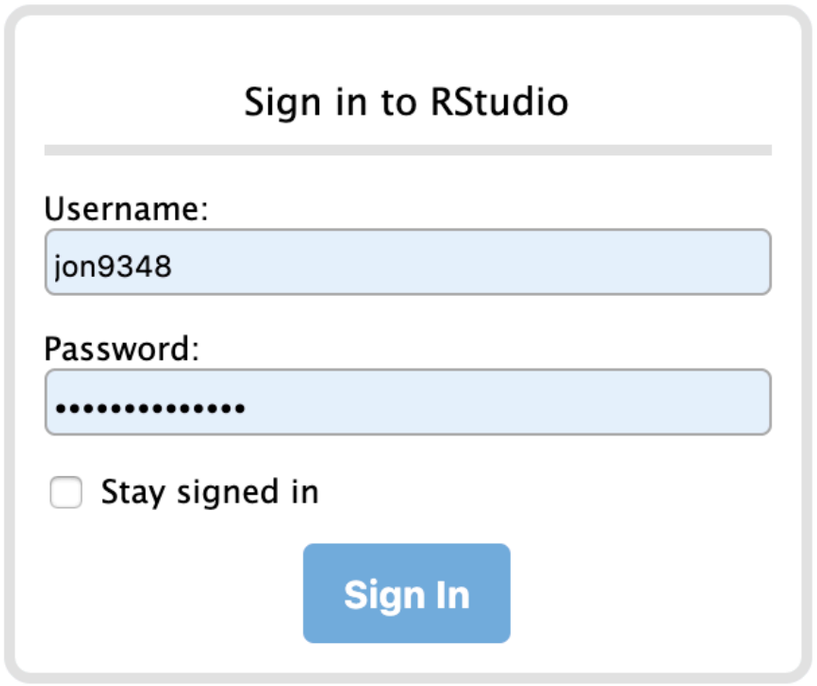
http://www.it.northwestern.edu/research/user-services/quest/genomics.html

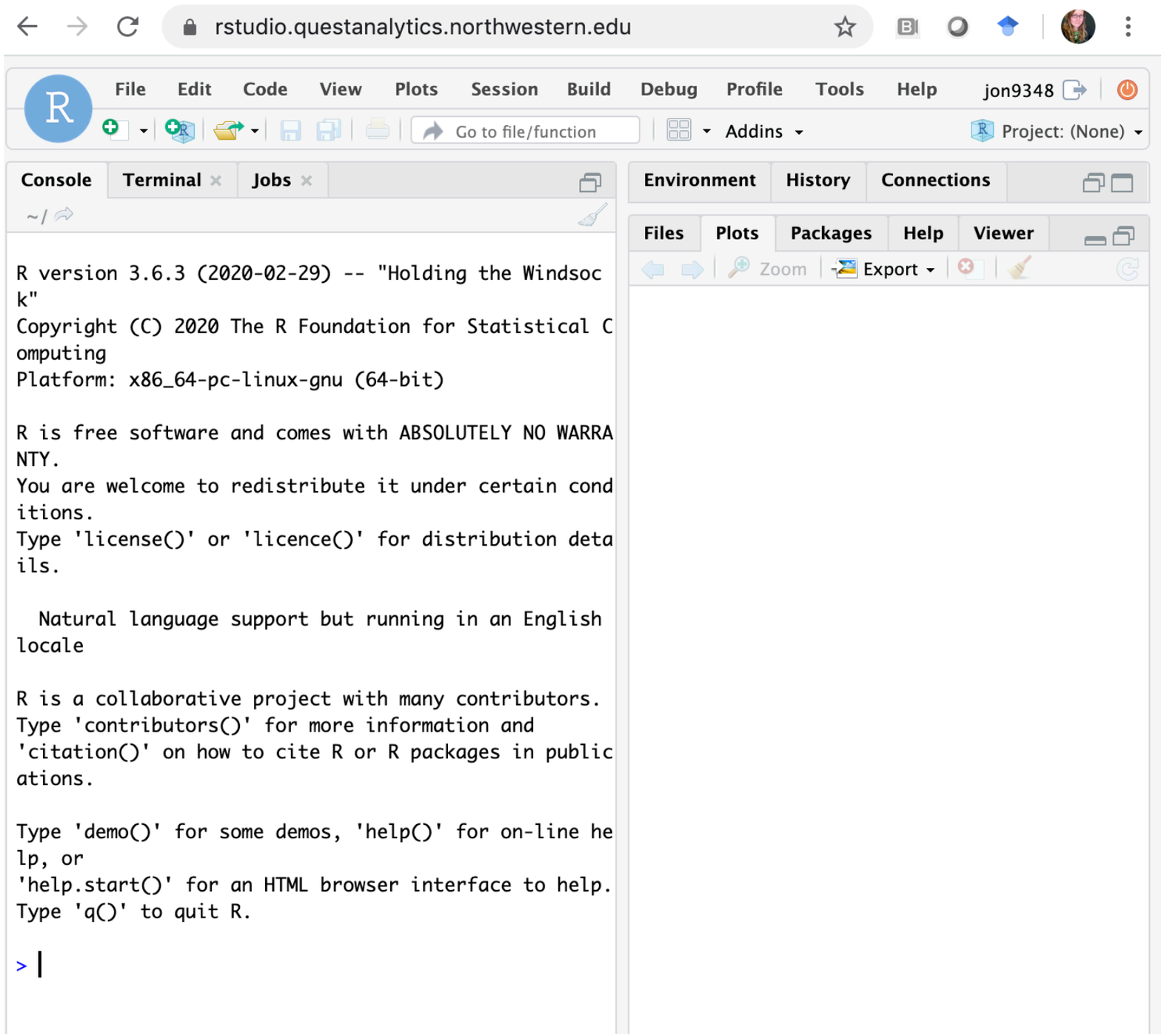
Analytics Nodes

The Quest Analytics Nodes allow users to run RStudio, Jupyter Notebooks and SAS Studio in their web browser, backed by Quest file systems and nodes with more computational resources than available on a personal computer. They are available to all Quest users with an active allocation.

https://rstudio.questanalytics.northwestern.edu

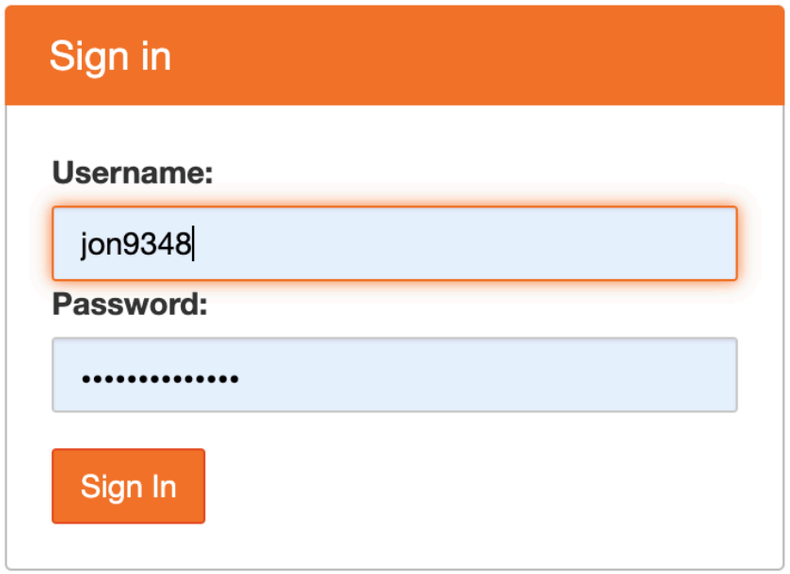
R 3.6.3

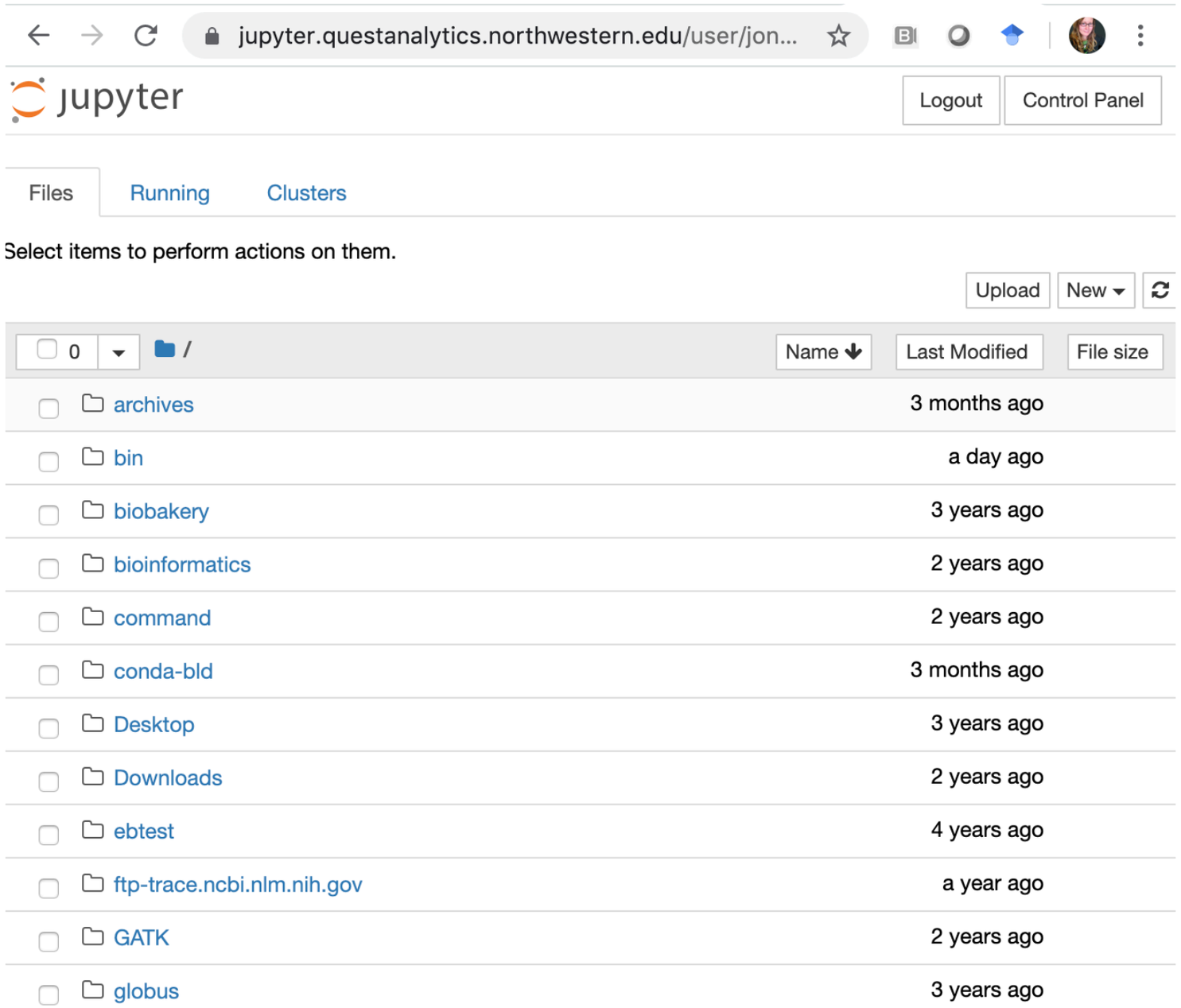




https://jupyter.questanalytics.northwestern.edu

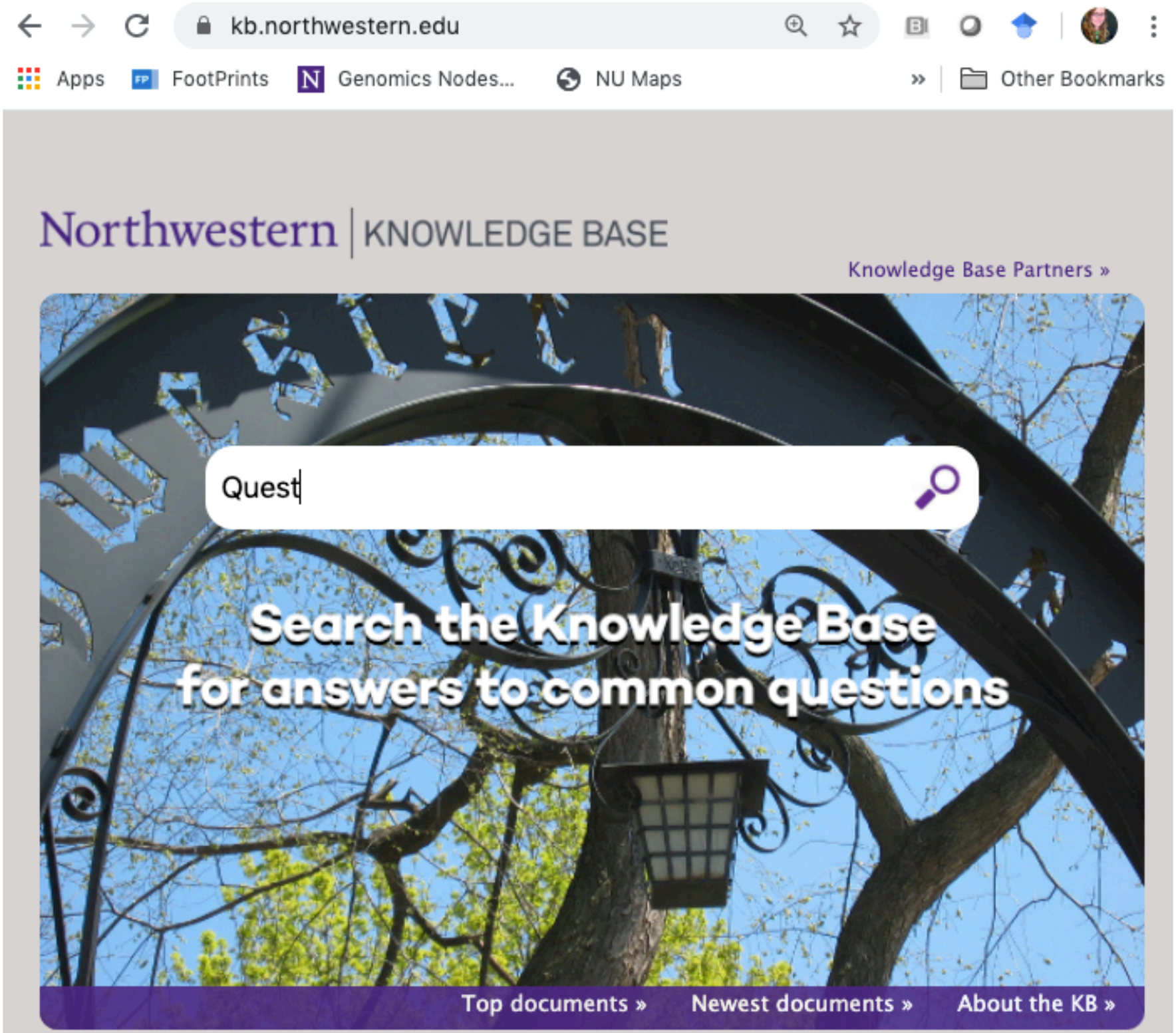
Python 3.7.1





High-Memory Nodes
GPU Nodes

kb.northwestern.edu
search for “Quest Partitions/Queues”


kb.northwestern.edu
Apps
FootPrints
Genomics Nodes...
NU Maps
Other Bookmarks
Northwestern | KNOWLEDGE BASE
Knowledge Base Partners »
Quest
Search the Knowledge Base
for answers to common questions
Top documents »
Newest documents »
About the KB »

kb.northwestern.edu/search.php?q=Quest

Apps | FootPrints | Genomics Nodes... | NU Maps | trainshuttle.pdf | Intercampus | Other Bookmarks

Northwestern | KNOWLEDGE BASE

Quest

All Audiences | SEARCH | Advanced

Keywords | 20 per page | Results: 1-20 of 46

Sort by relevance | XML | JSON | OL

No.	Document Title	ID	Updated	Hits
1	**** Quest User Guide	72406	2020-03-05	61512
2	*** Quest Quick Start Guide	70706	2019-11-18	44921
3	Quest FAQ	90865	2019-12-20	3040
4	Transferring Files to and from Quest	70521	2019-11-11	24034
5	Using MATLAB on Quest	70716	2019-06-06	12227
6	Connecting to Quest with FastX	69237	2019-09-04	26378
7	Using Jupyter on the Quest Analytics Nodes	94116	2020-03-05	2121
8	Quest Beta Cluster	93847	2019-09-04	1217
9	Using RStudio on the Quest Analytics Nodes	71895	2019-08-27	17289
10	Using SAS Studio on the Quest Analytics Nodes	76583	2019-04-15	12287
11	Getting Started on the Genomics Compute Cluster (b1042) on Quest	78602	2019-04-23	8821
12	Troubleshooting Installing R Packages on Quest and Quest Analytics	98203	2020-04-06	256

Backing up your data

Northwestern Box: unlimited, free, 15GB single file limit

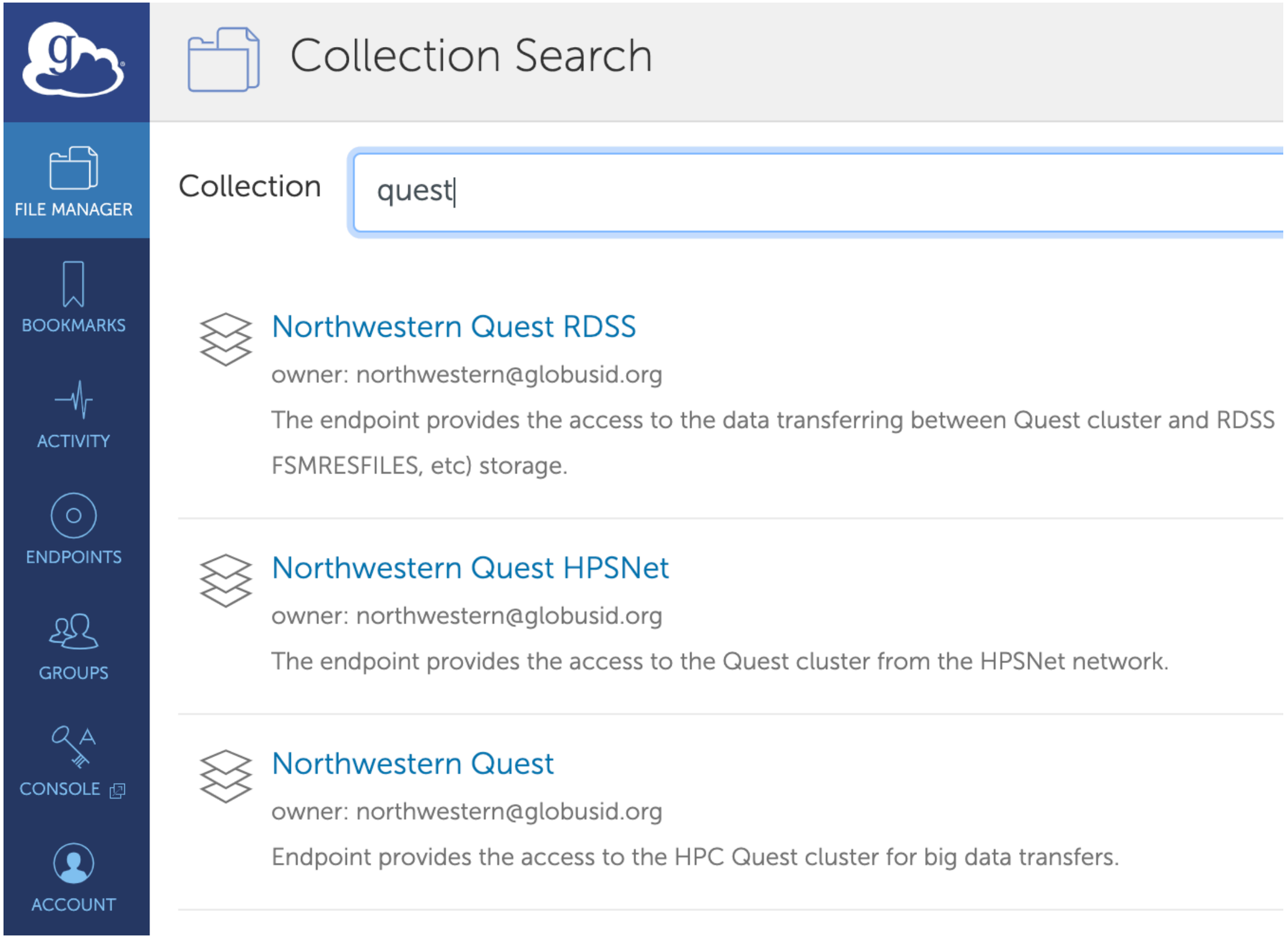
RDSS (Research Data Storage Service)
& FSMRESfiles (for Feinberg research)

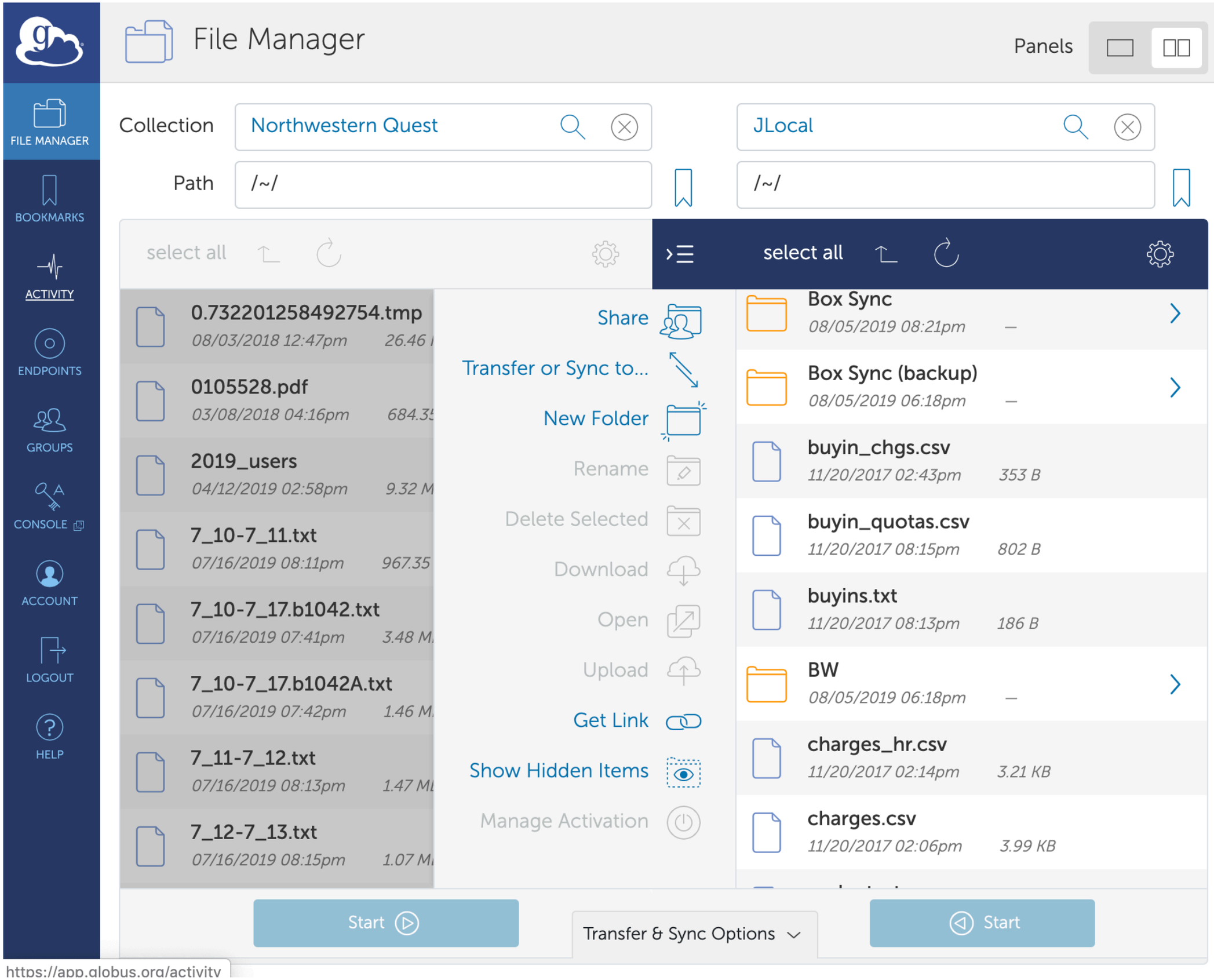
Amazon AWS

Other cloud options

globus.org


globus.org
globus
a uchicago non-profit service
I Want To...
Pricing
Resources
Support
About
Log In
JOIN US FOR
GlobusWorld 2020
A Virtual Event on April 29, 2020
VISIT GLOBUSWORLD.ORG TO LEARN MORE
10 YEARS
Research data management simplified.
TRANSFER
SHARE
BUILD


Collection Search
FILE MANAGER
BOOKMARKS
ACTIVITY
ENDPOINTS
GROUPS
CONSOLE
ACCOUNT
Collection
quest
Northwestern Quest RDSS
owner: northwestern@globusid.org
The endpoint provides the access to the data transferring between Quest cluster and RDSS
FSMRESFILES, etc) storage.
Northwestern Quest HPSNet
owner: northwestern@globusid.org
The endpoint provides the access to the Quest cluster from the HPSNet network.
Northwestern Quest
owner: northwestern@globusid.org
Endpoint provides the access to the HPC Quest cluster for big data transfers.

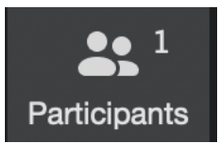

File Manager
Panels
FILE MANAGER
BOOKMARKS
ACTIVITY
ENDPOINTS
GROUPS
CONSOLE
ACCOUNT
LOGOUT
HELP
Collection
Northwestern Quest
JLocal
Path
/~/
/~/
select all
select all
0.732201258492754.tmp
08/03/2018 12:47pm
0105528.pdf
03/08/2018 04:16pm
2019_users
04/12/2019 02:58pm
7_10-7_11.txt
07/16/2019 08:11pm
7_10-7_17.b1042.txt
07/16/2019 07:41pm
7_10-7_17.b1042A.txt
07/16/2019 07:42pm
7_11-7_12.txt
07/16/2019 08:13pm
7_12-7_13.txt
07/16/2019 08:15pm
Share
Transfer or Sync to...
New Folder
Rename
Delete Selected
Download
Open
Upload
Get Link
Show Hidden Items
Manage Activation
Box Sync
08/05/2019 08:21pm
Box Sync (backup)
08/05/2019 06:18pm
buyin_chgs.csv
11/20/2017 02:43pm
353 B
buyin_quotas.csv
11/20/2017 08:15pm
802 B
buyins.txt
11/20/2017 08:13pm
186 B
BW
08/05/2019 06:18pm
charges_hr.csv
11/20/2017 02:14pm
3.21 KB
charges.csv
11/20/2017 02:06pm
3.99 KB
Start
Transfer & Sync Options
Start
https://app.globus.org/activity

BREAK

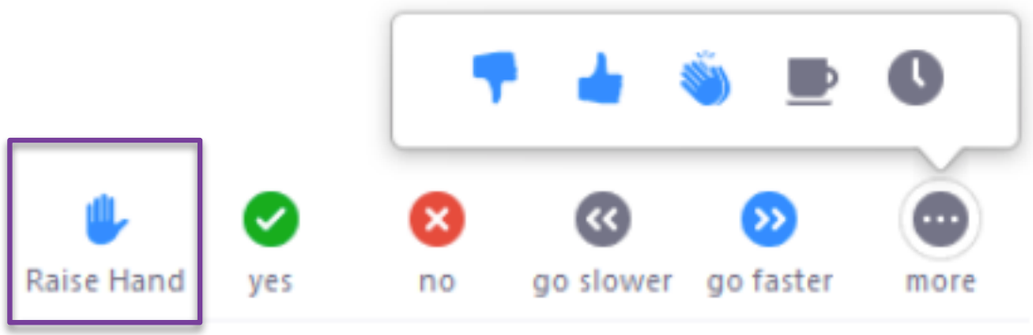
Please set up your screen to have Zoom on one half of the screen and a terminal or web browser on the other half.

“Raise Hand”

Click here →



Click →



Getting Started: Batch Job Submission

What is the scheduler looking for in your script?

Behold, this is a BASH script: `#!/bin/bash`

Account: `#SBATCH -A p20XXX`

Partition/Queue: `#SBATCH -p short`

Number of nodes: `#SBATCH –N 1`

Number of cores: `#SBATCH –ntasks-per-node=1`

Length of the job: `#SBATCH –t 04:00:00`

Required memory: `#SBATCH --mem-per-cpu=1G`

Name of the job: `#SBATCH -J sample_job`

Generate an output log: `#SBATCH -o outlog`

Generate an error log: `#SBATCH -e errlog`

Getting Started: Batch Job Submission

submit_generic_slurm.sh

```
#!/bin/bash
#SBATCH --account=<allocationID> ## <-- EDIT THIS TO BE YOUR ALLOCATION
#SBATCH --partition=<queue_type> ## <-- EDIT THIS TO BE YOUR partition NAME
#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 --error=errlog

module purge all        ## Unload existing modules
module load python      ## Load necessary modules (software, libraries)

bash whereami           ## Run the program
python helloworld.py    ## Run the program
```

Which partition should you use?

If your Allocation:

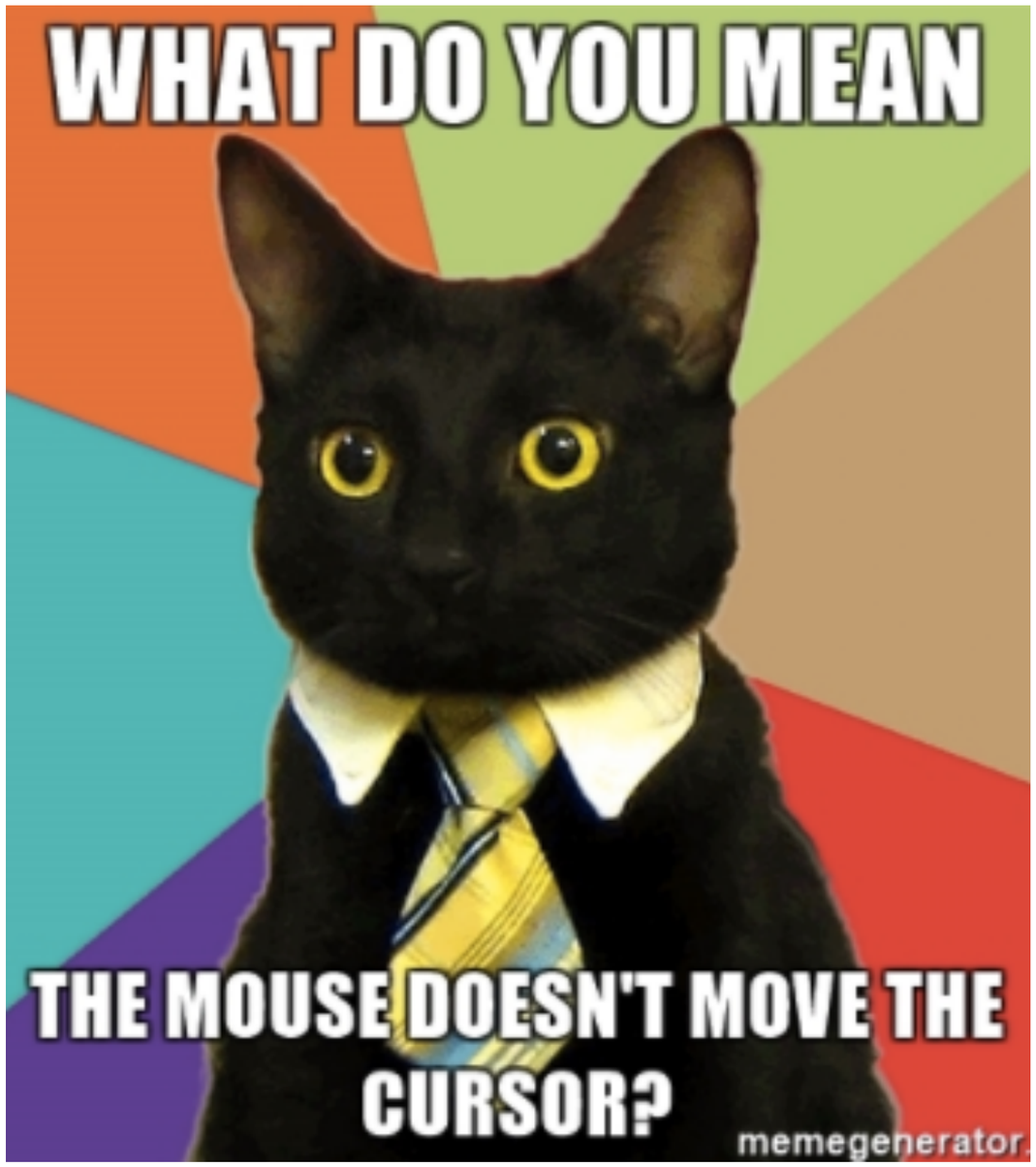
- starts with “**p**” or “**e**” use “**short**”
- starts with “**b**” use your Allocation name

  for example, for b1000 use partition “b1000”
- is “**b1042**” use “**genomics**”
- is “**w10001**” use “**w10001**”

Getting Started: Batch Job Submission

text editor: nano

- $ nano submit_generic_slurm.sh
  this will open the named file for editing or create it if it doesn't exist
- type your text: the mouse will not move the cursor - navigate with the arrow keys
- save and quit: commands are on the bottom of the screen - the "^" stands for "control"



Interactive on Quest

Questions?

Help email: quest-help@northwestern.edu

Research Computing Services

Northwestern
INFORMATION TECHNOLOGY

Python package installation

`$ module load python`

This will load a development level version of python (2.7) in your environment

`$ pip install –user tensorflow –upgrade`

Install the package - check in **`/home/netID/.local`**

Start python and to test type : **`import tensorflow as tf`**

You can exit python by typing: **`quit()`** and press enter

R package installation

$ module load R/3.4.3

This will load a development level version of R (3.4.3) in your environment

$ R (*enter the R interpreter environment*)

> install.packages('tensorflow')

You can click yes to all the options

Check by typing: **library('tensorflow')**

Exit by typing: **quit()** and then type **n (for no)**

Installations will be in home directory under: **/home/netid/R/x86_64-pc-linux-gnu-library/3.4/**

Build your own package/libraries: fftw

Create a directory and download:

$ **mkdir csr; cd csr; wget http://www.fftw.org/fftw-3.3.7.tar.gz**

Unpack: $ **tar -xvmf fftw-3.3.7.tar.gz**

Enter package directory, configure and build

$cd fftw-3.3.7 ; ./configure -prefix=/home/netID/fftw_install ; make ; make install

Inspect installation: $ **ls fftw_install**

Installation contains directories **bin include lib share**

Add environmental variables in your **/home/netID/.bashrc** file:

```
export $PATH=/home/netID/fftw_install/bin:$PATH
export $LD_LIBRARY_PATH=/home/netID/fftw_install/lib:$LD_LIBRARY_PATH
export $PKG_CONFiG_PATH=$LD_LIBRARY_PATH/pkgconfig:$PKG_CONFIG_PATH
```

Build your code

Download a sample code that needs your libraries

```
$ wget http://geco.mines.edu/files/userguides/techReports/mklWrappers/fft_example/test.c
```

Compile:

```
$ gcc test.c -o test \
-L$HOME/fftw_install/lib -
-I$HOME/fftw_install/include
```

Compiler-Source-Exec

Linking to libraries &headers

Run:

```
./test >& output
```