

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

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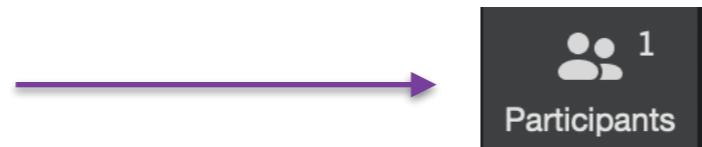
How this workshop will work

- 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

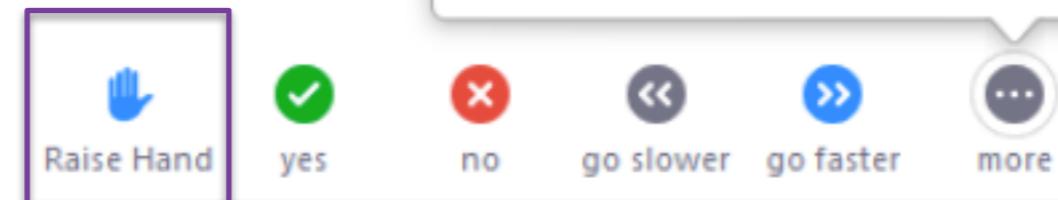
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“Raise Hand” if you don’t have a Quest account

Click here



Click



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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

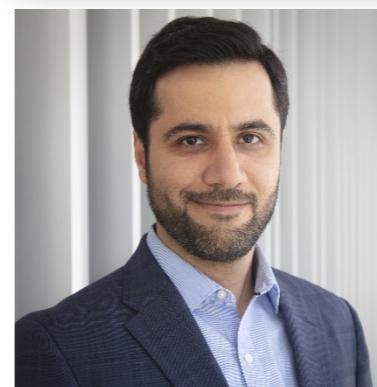
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Research Computing: the Consultants

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



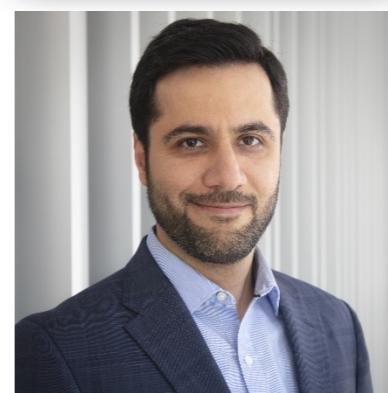
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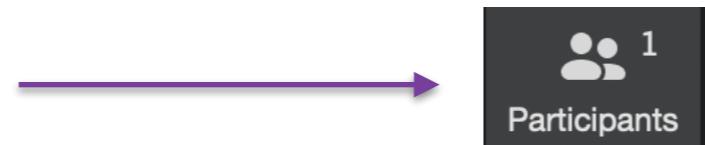
Janna Nugent



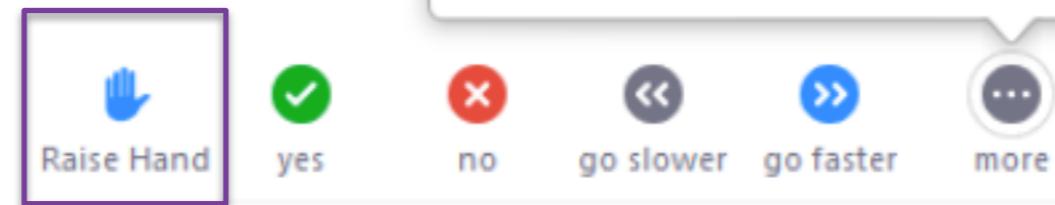
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Click



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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



The login page features the FAST logo at the top center. Below it are fields for 'User Name' and 'Password'. A checkbox labeled 'Use Public Key Authentication' is present, with a link 'Manage Private Keys' below it. A large blue 'Log In' button is at the bottom. Smaller links for 'Admin Login' and 'Build: 2.4.15' are located at the bottom right.

User Name

Password

Use Public Key Authentication

[Manage Private Keys](#)

[Log In](#)

[Admin Login](#)

Build: 2.4.15

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

Login to Quest

http://quest.northwestern.edu:3000



User Name
jon9348|

Password
.....

Use Public Key Authentication
[Manage Private Keys](#)

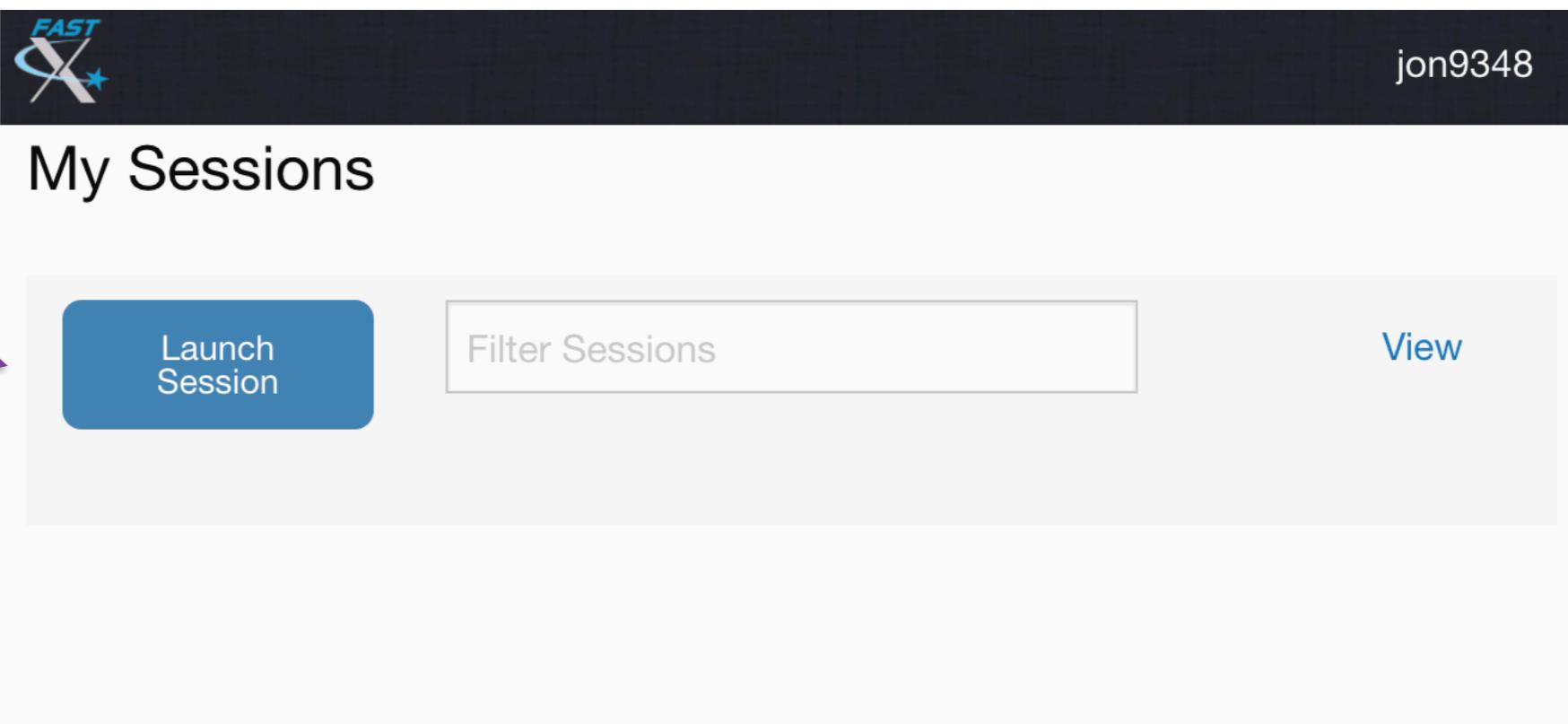
Log In

[Admin Login](#)
Build: 2.4.15

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

Login to Quest

http://quest.northwestern.edu:3000



The screenshot shows the Quest login interface. At the top, there is a dark header bar with the FAST logo on the left and the user ID "jon9348" on the right. Below the header, the main page title "My Sessions" is displayed. Underneath the title are three buttons: a blue "Launch Session" button with white text, a grey "Filter Sessions" input field, and a blue "View" button with white text. A purple arrow points from the text "Click" on the left towards the "Launch Session" button.

Click

Launch Session

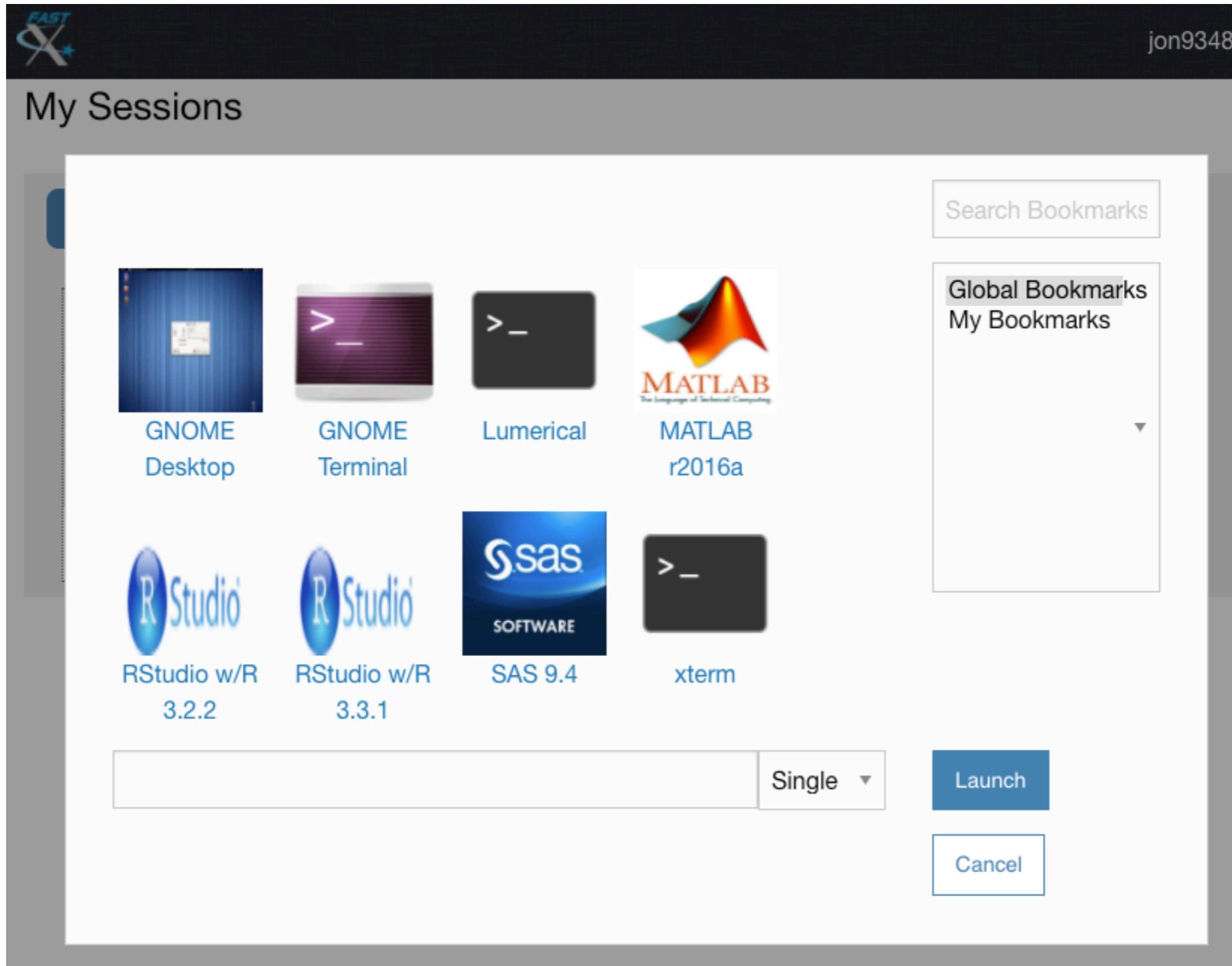
Filter Sessions

View

Click the “Launch Session” button

Login to Quest

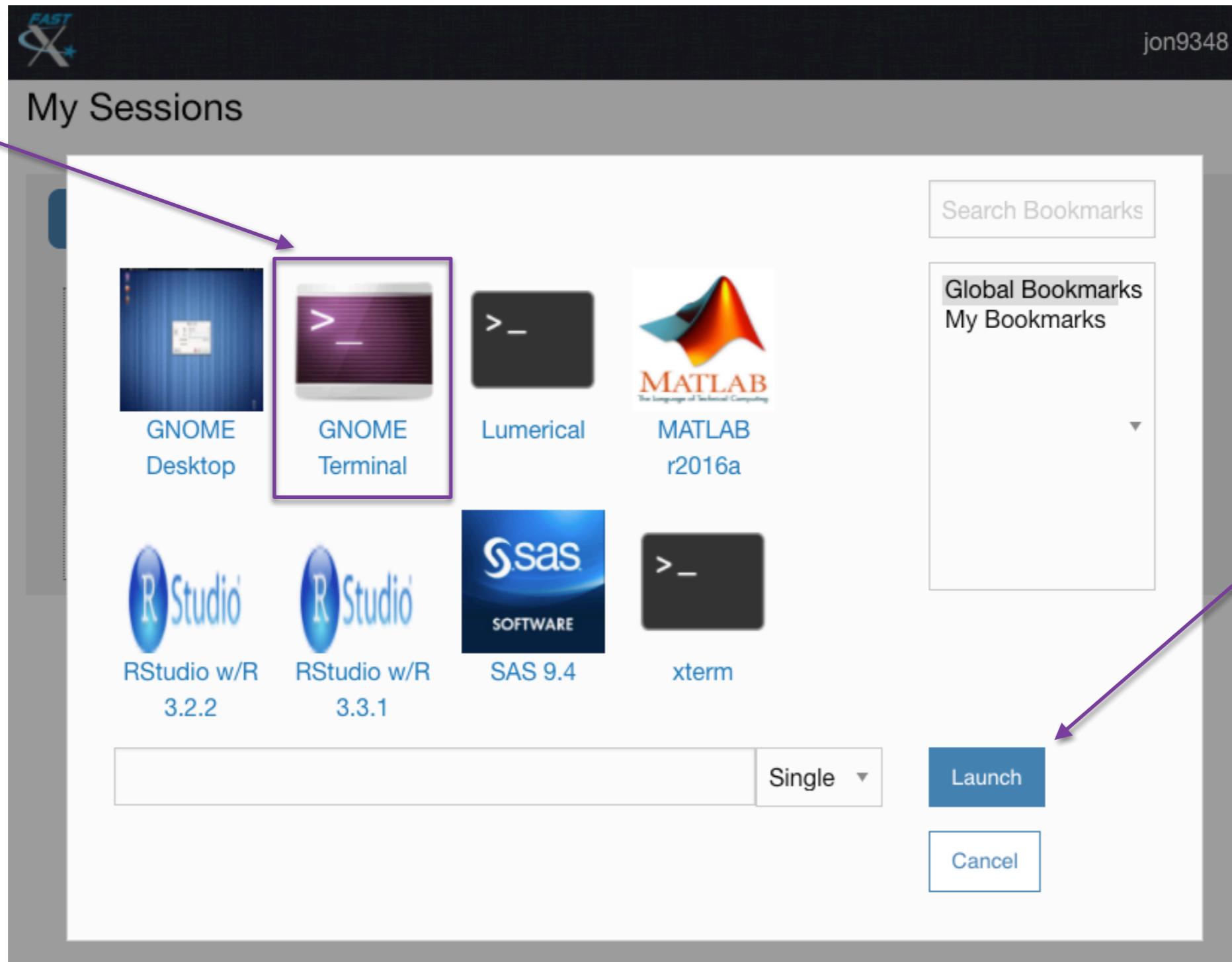
<http://quest.northwestern.edu:3000>



Login to Quest

<http://quest.northwestern.edu:3000>

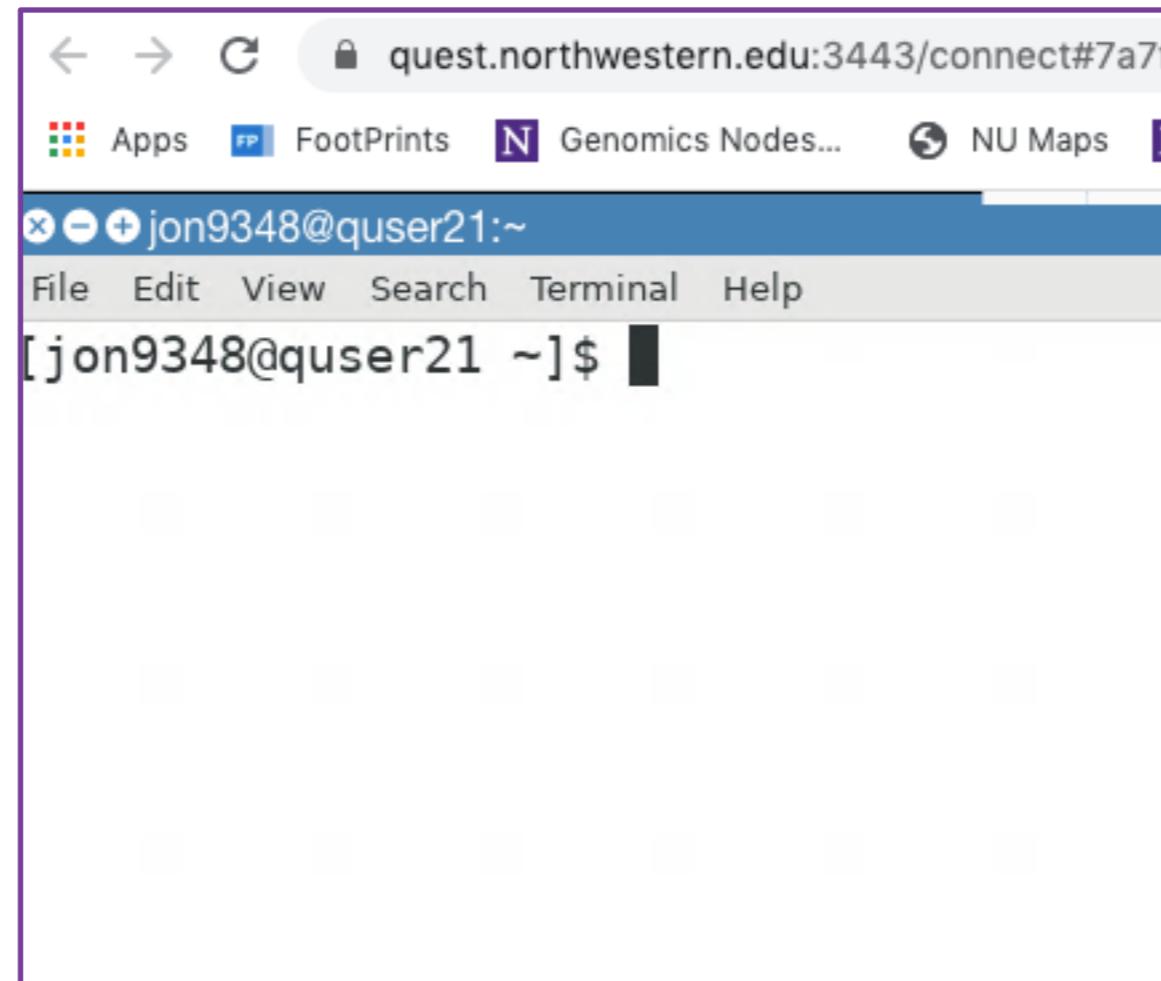
1) Select



2) Click

Login to Quest

http://quest.northwestern.edu:3000

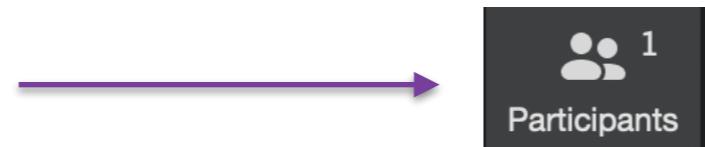


Success!

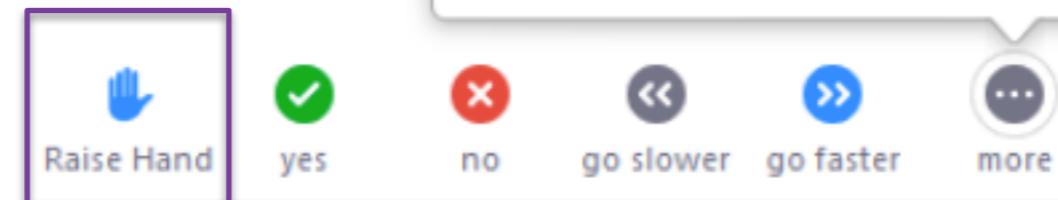
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**“Raise Hand” if you
can’t login**

Click here



Click



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

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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 ~]\$

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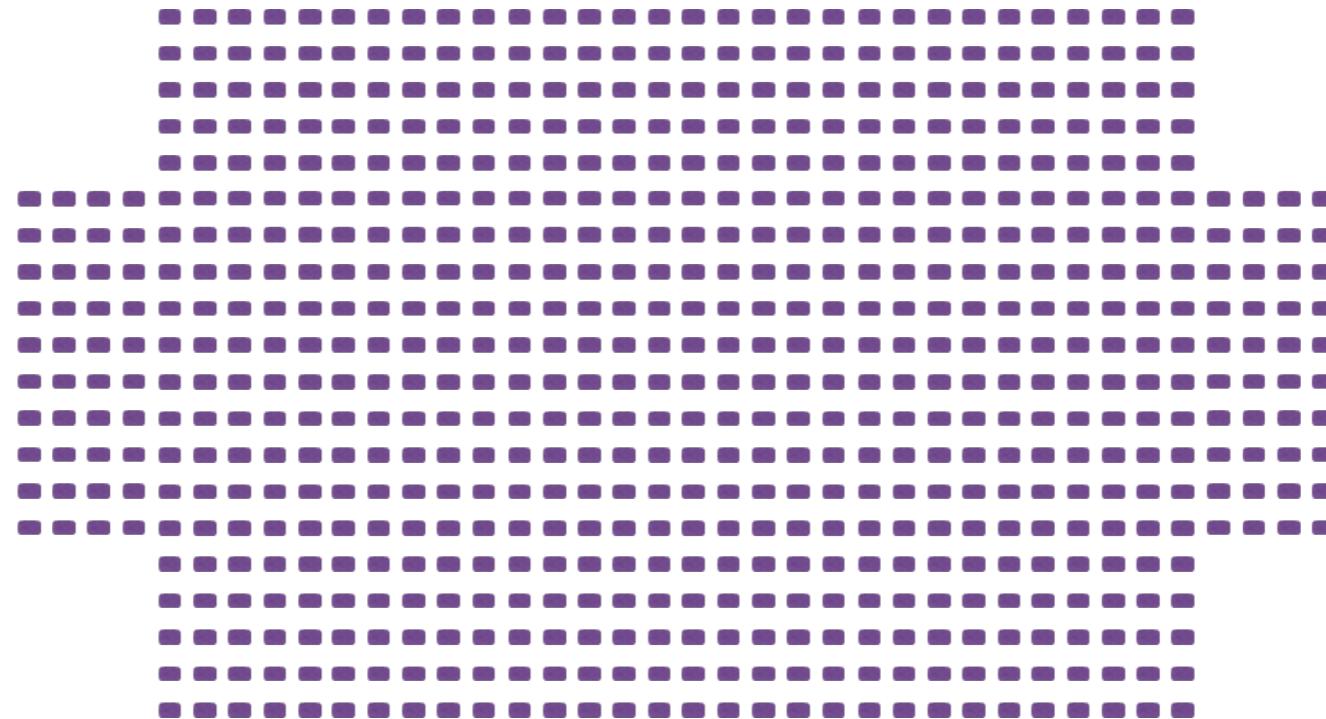
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[jon9348@quser22 ~]\$

high-performance compute cluster

high-performance compute cluster

750 computers



high-performance compute cluster

computer = “node”



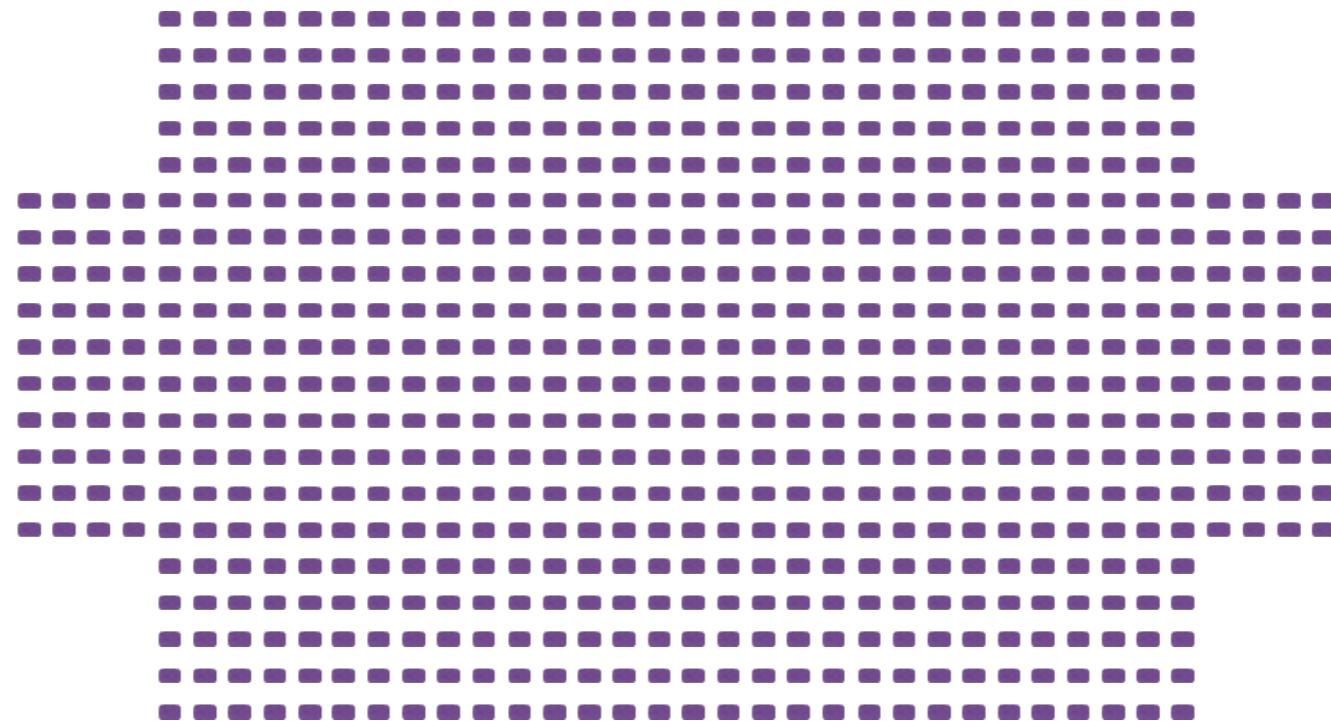
nodes in racks

high-performance compute cluster



high-performance compute cluster

750 nodes



high-performance compute cluster

1

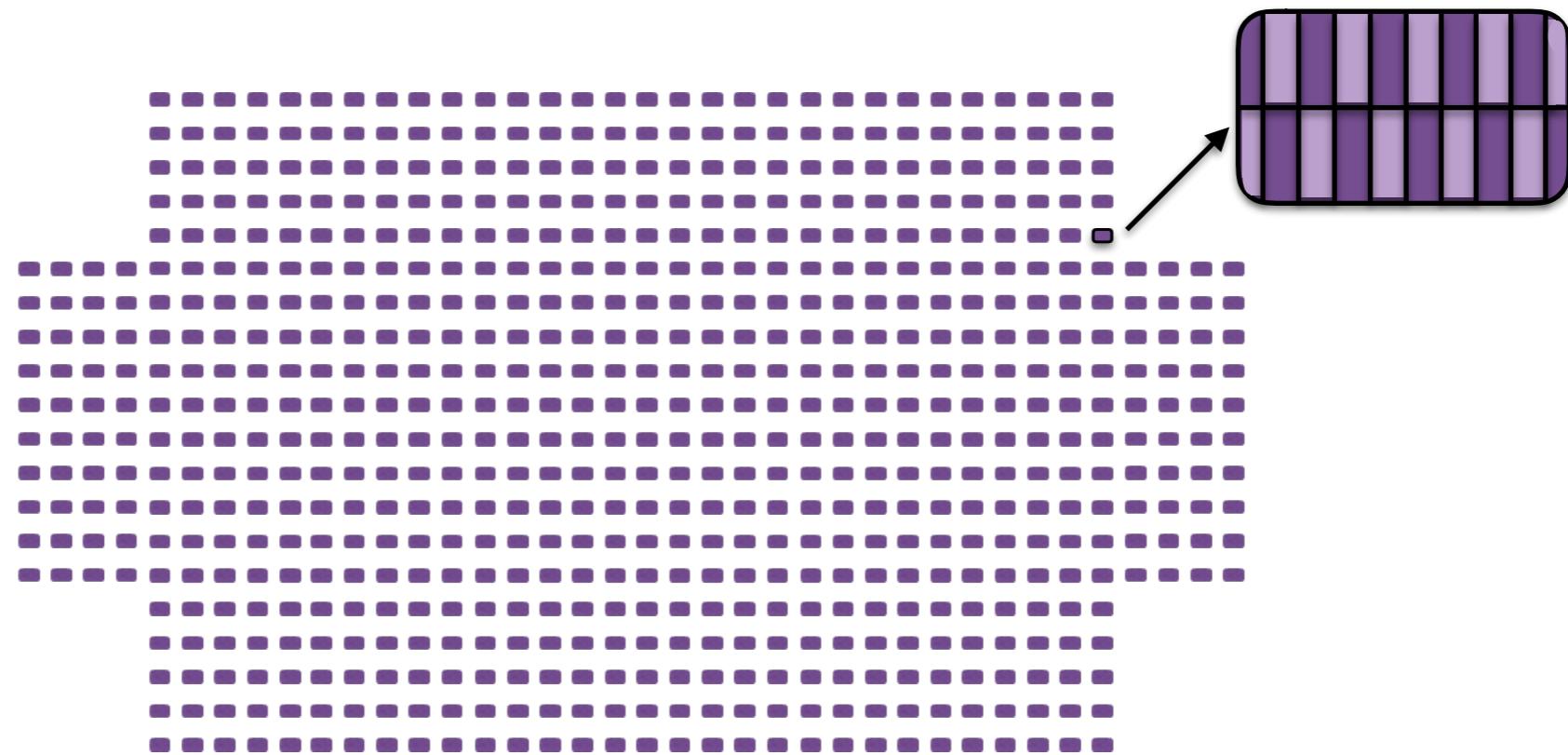
750

	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

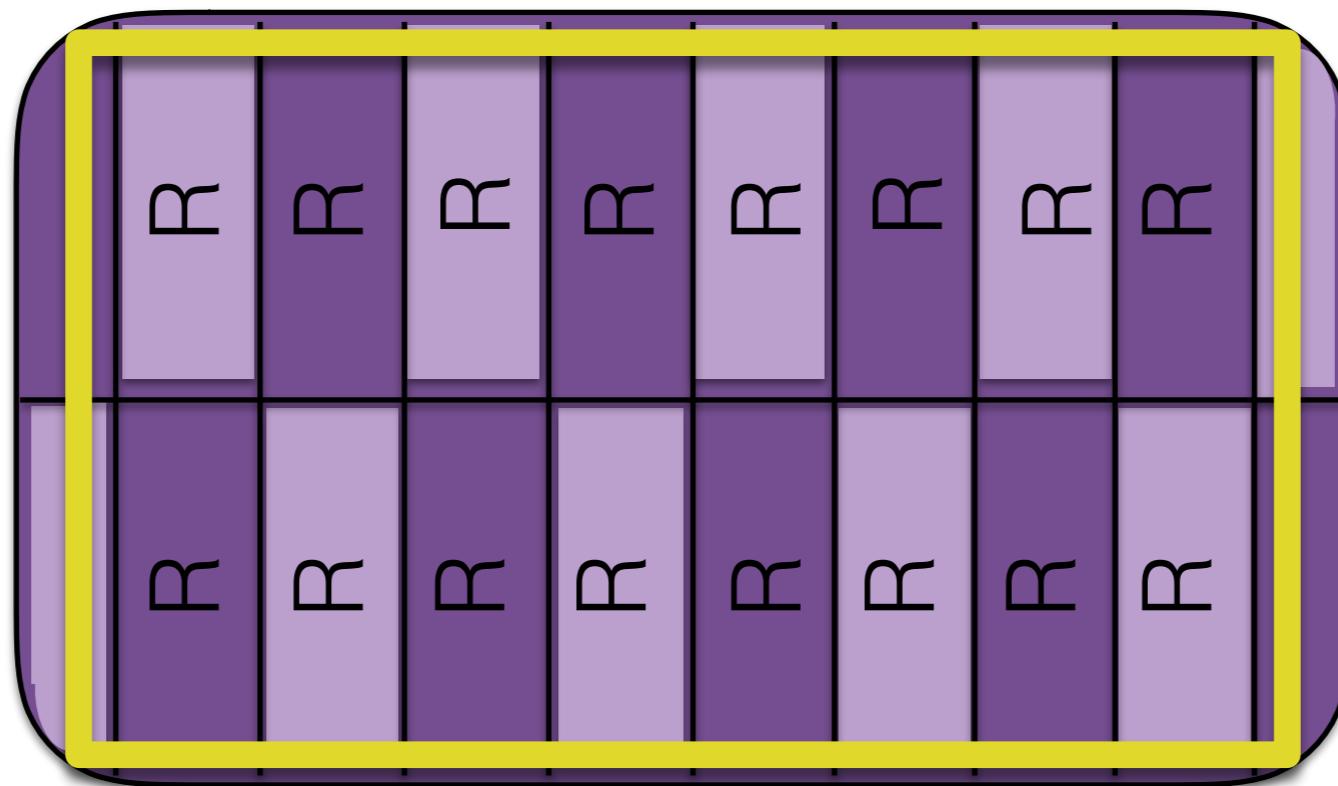
Each node can run **jobs** from
24-40 researchers at once



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

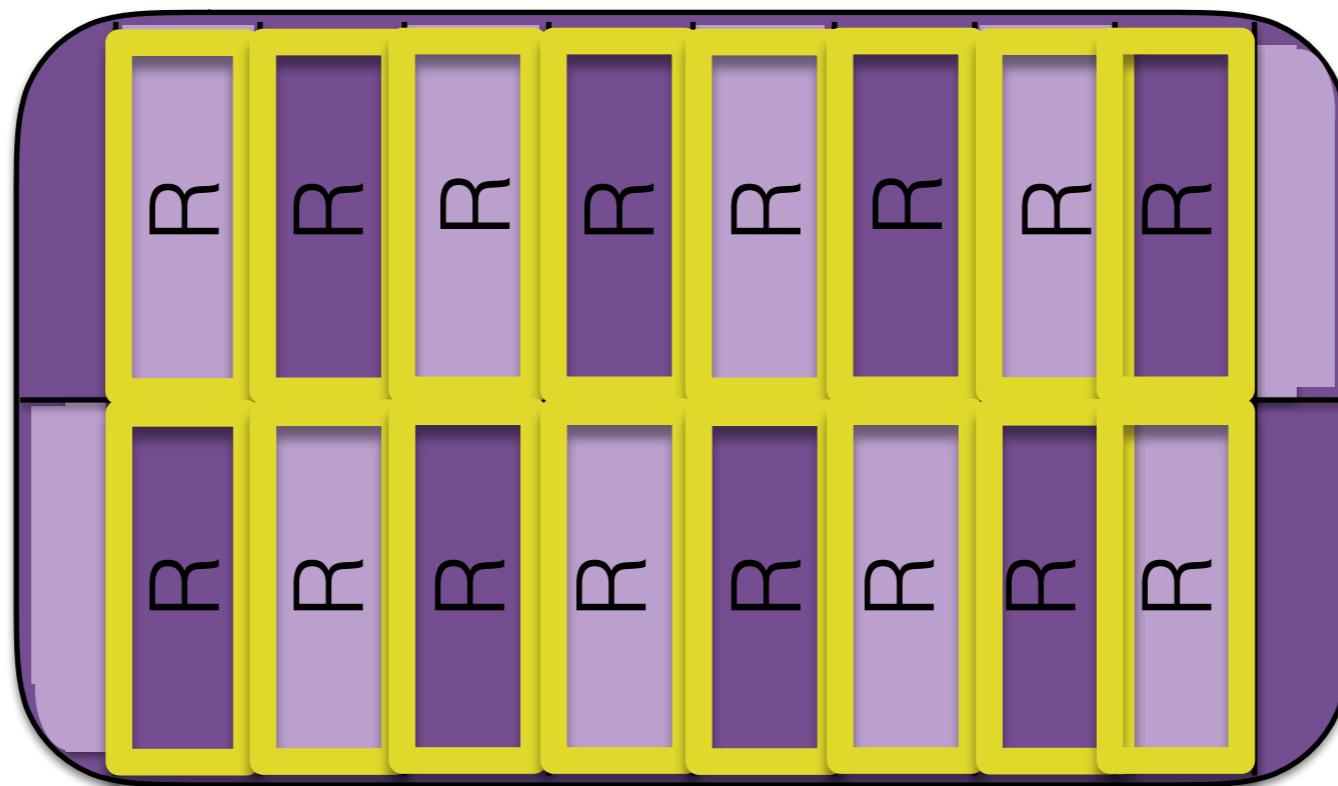
high-performance compute cluster

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



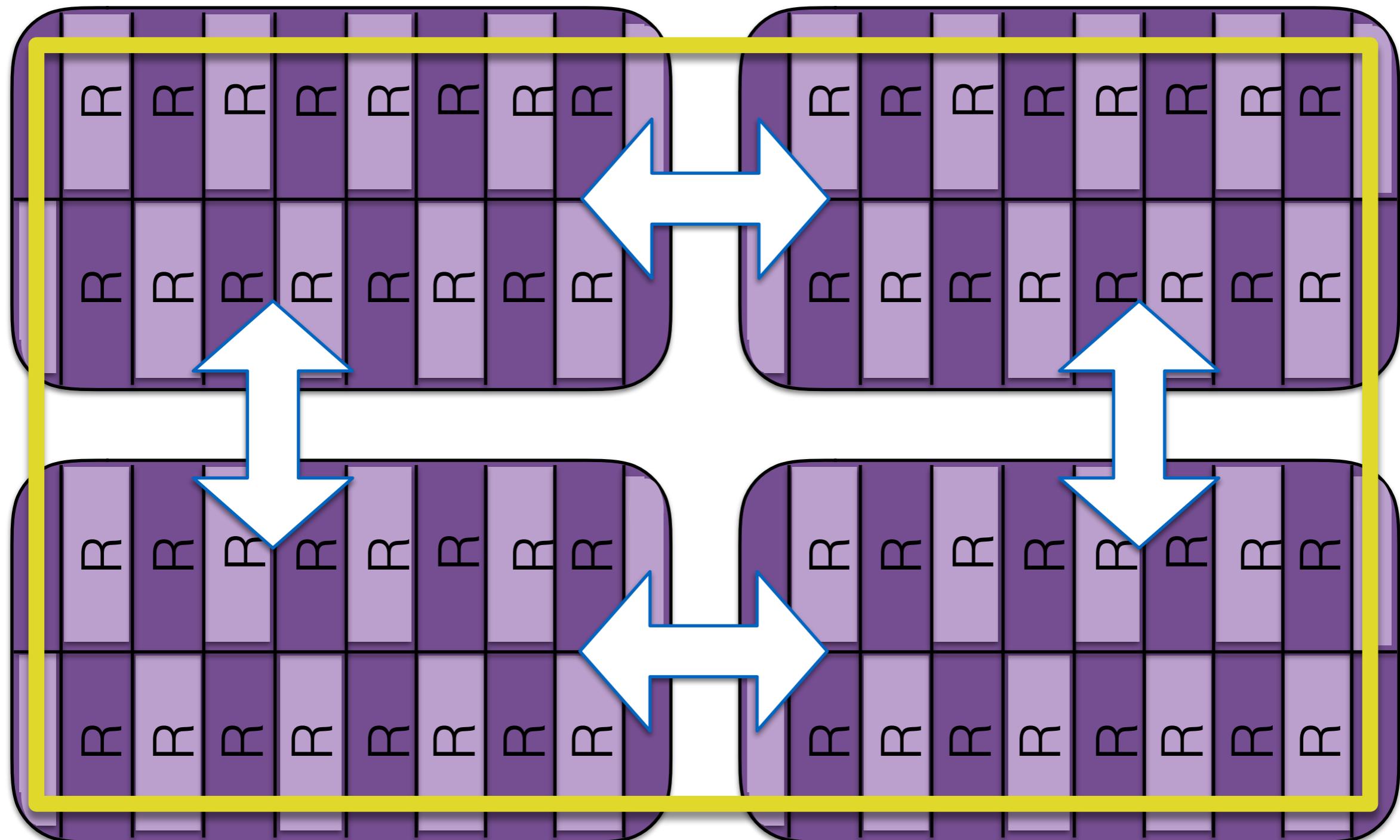
high-performance compute cluster

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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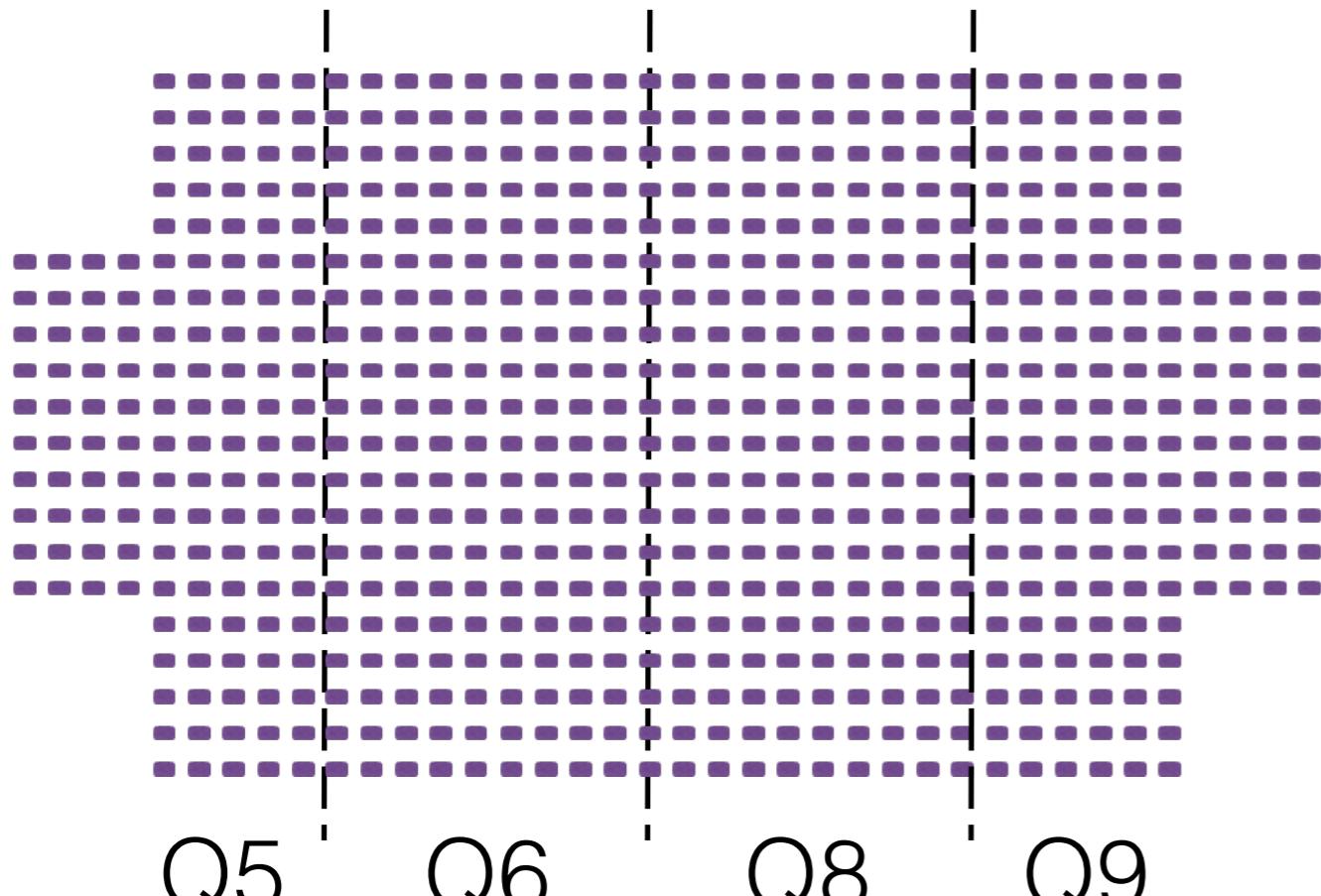
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[jon9348@quser22 ~]\$

high-performance compute cluster

Node Architectures: 4 Generation of Nodes



- 128 GB RAM (Q5, Q6)
- 96 GB RAM (Q8)
- 192 GB RAM (Q9)
- $Q5 \rightarrow 24 \text{ cores/node}$
- $Q6 \rightarrow 28 \text{ cores/node}$
- $Q8 \rightarrow 28 \text{ cores/node}$
- $Q9 \rightarrow 40 \text{ cores/node}$

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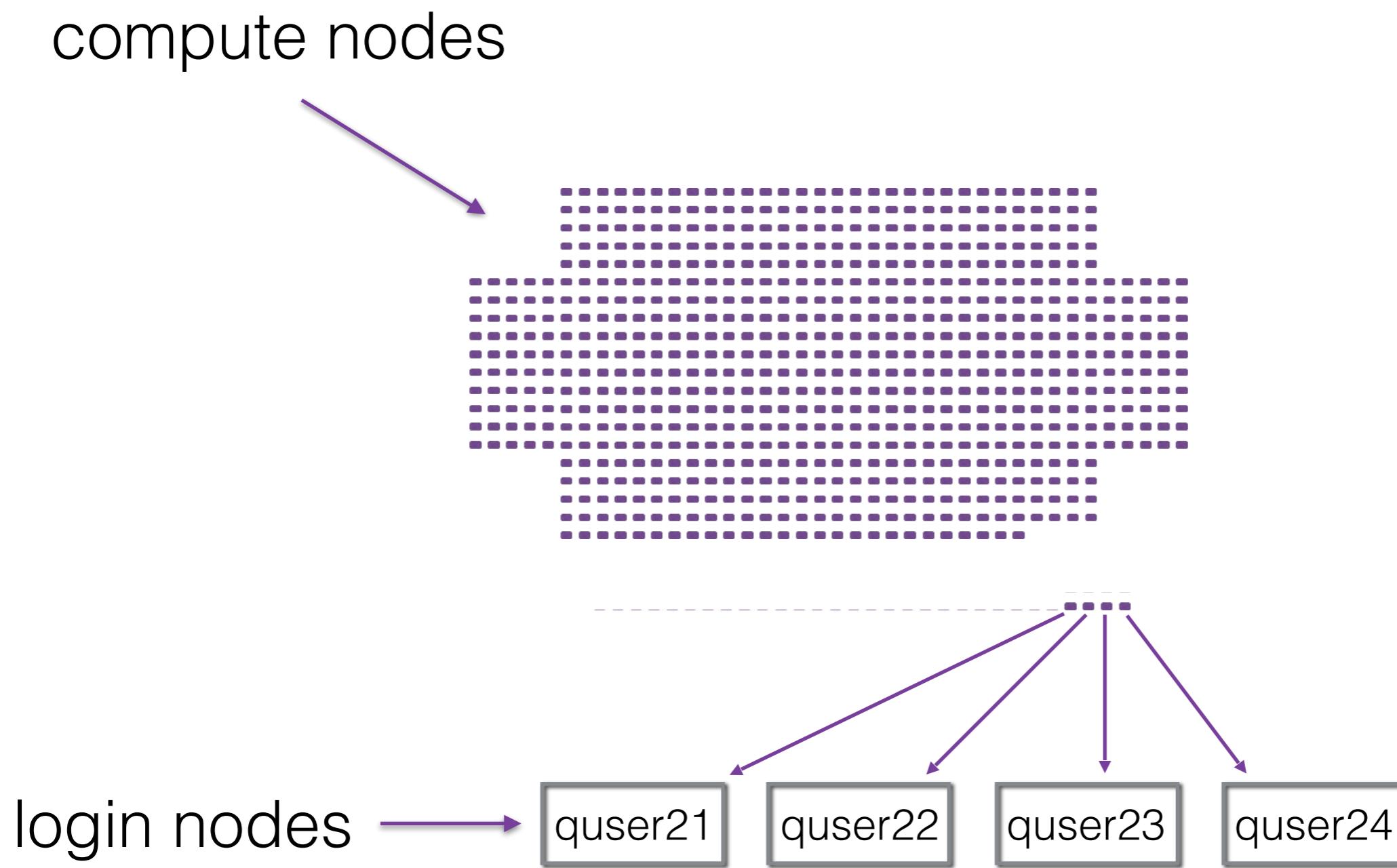
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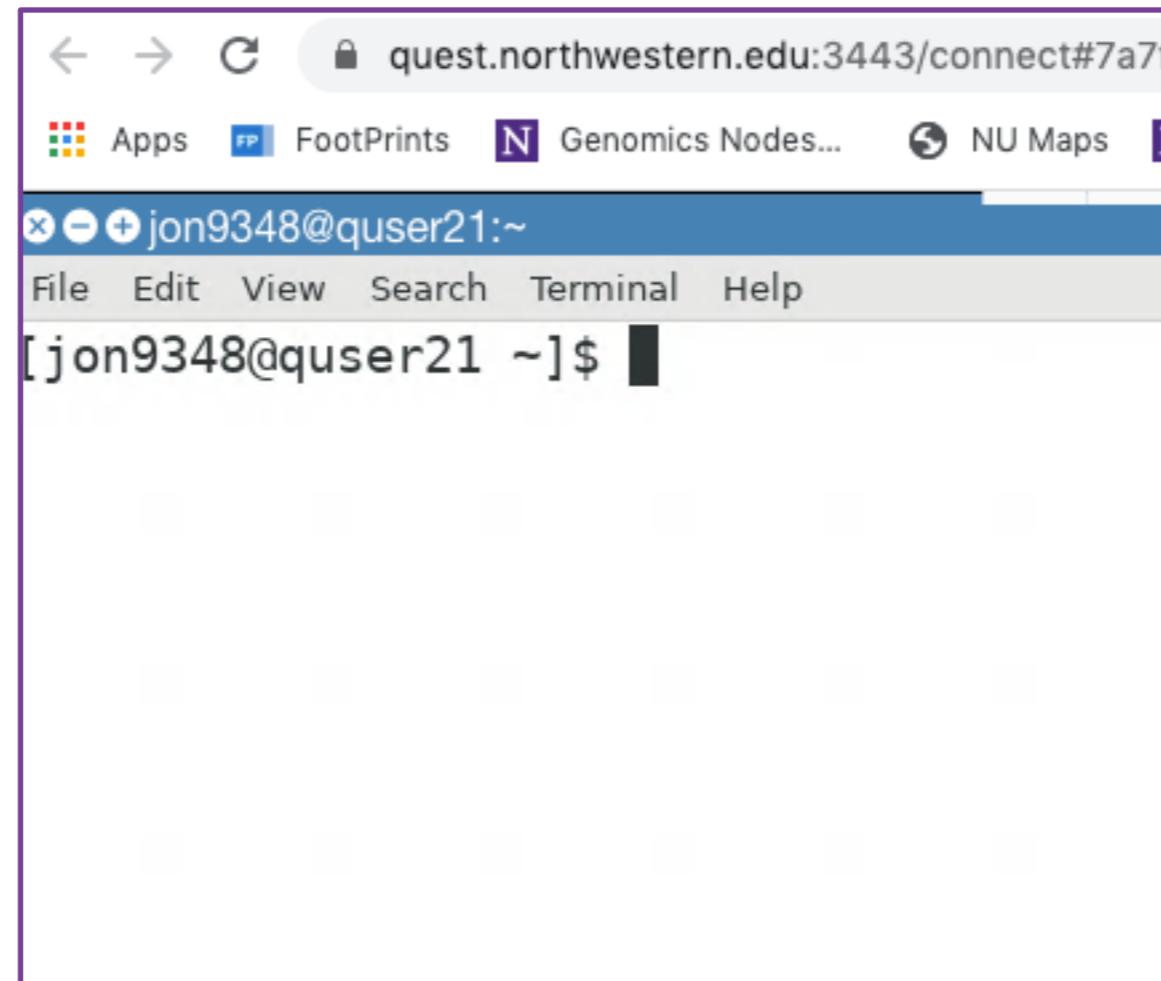
[jon9348@quser22 ~]\$

Quest: High Performance Compute Cluster



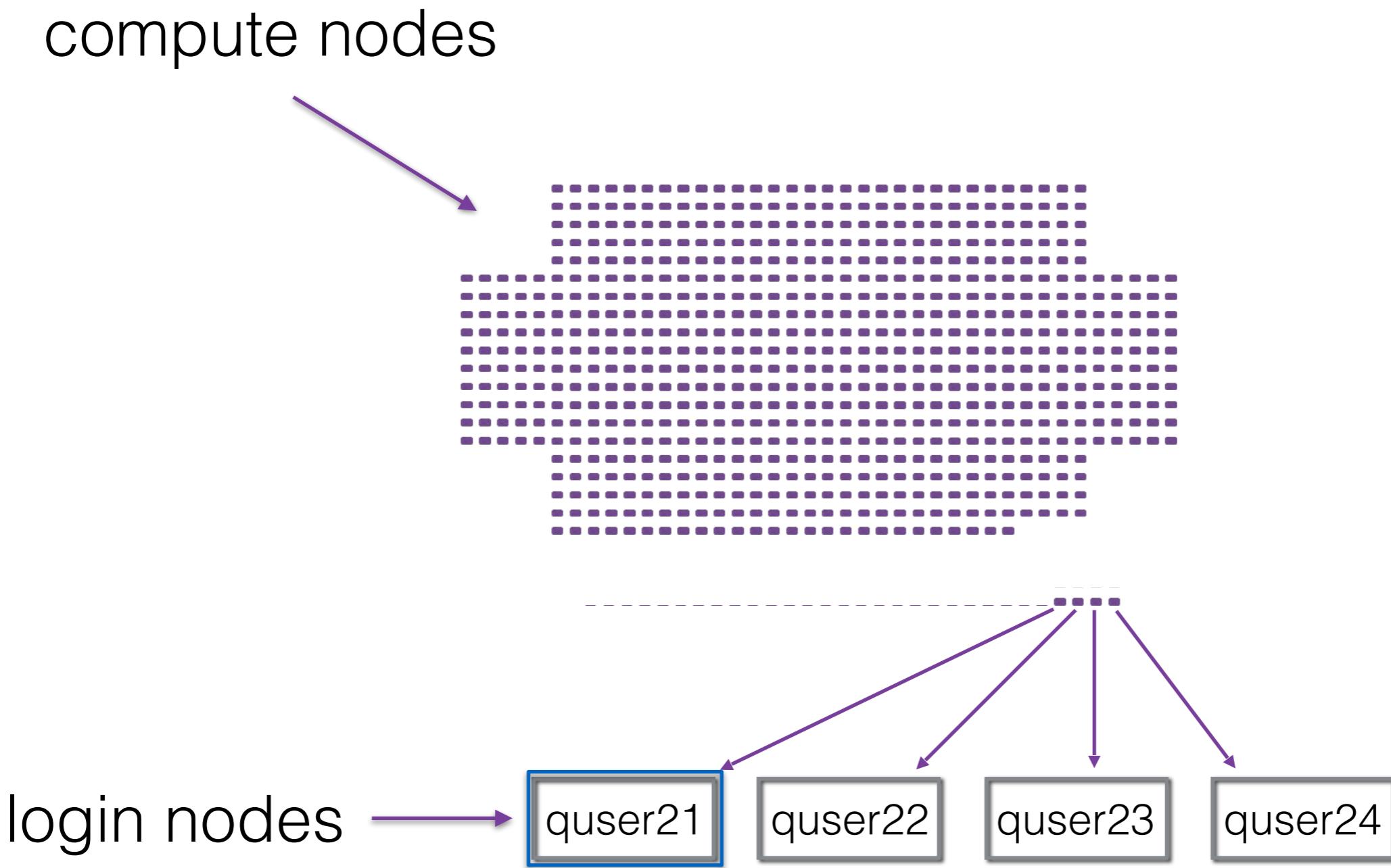
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http://quest.northwestern.edu:3000



Success!

Quest: High Performance Compute Cluster



Interactive on Quest

BREAK

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[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

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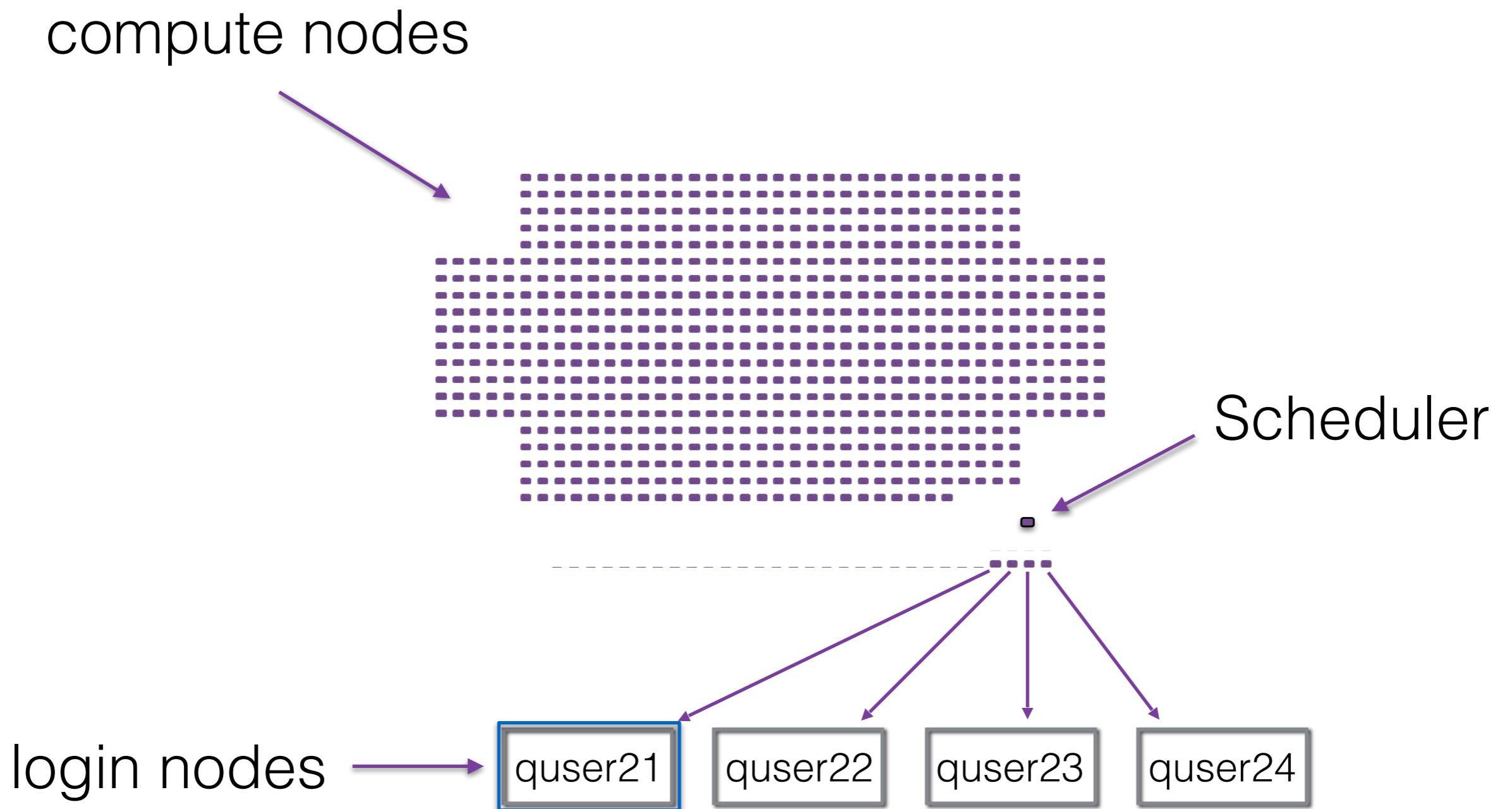
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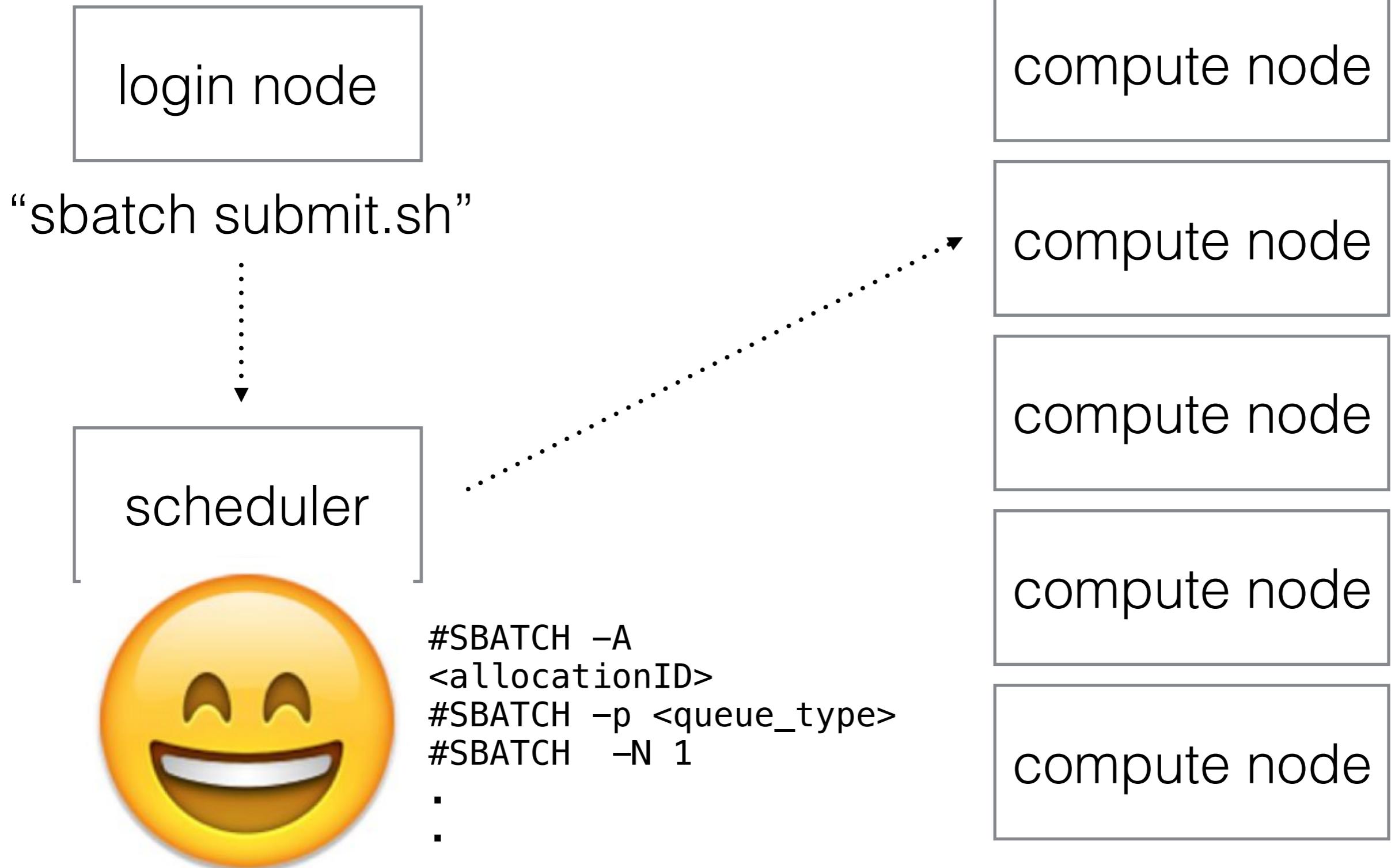
[jon9348@quser22 ~]\$

Interactive on Quest

Quest: High Performance Compute Cluster



The Scheduler



Account vs. Allocation

Account

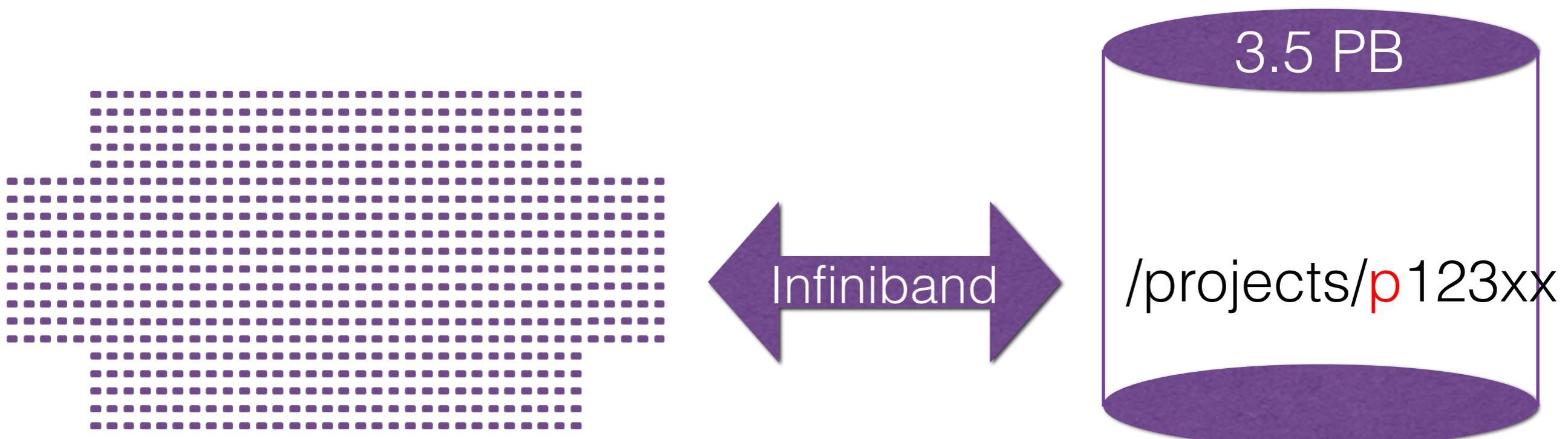
- Private
 - `/home/<netID>`
 - Backed up
 - 80Gb storage quota

Allocation

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

Allocation Types: General Access

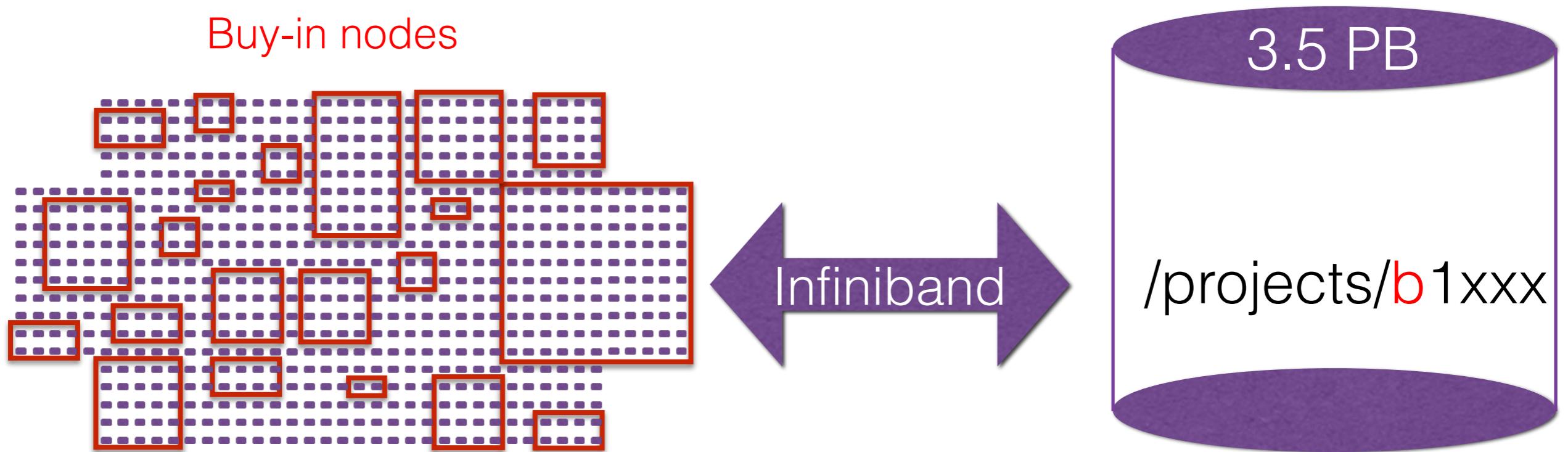
Research I Allocation, 500GB storage	computational need < 100K hour
Research II Allocation, 2TB storage	computational need > 100K hour
Classroom Allocation, 500GB storage	computational need < 100K hour



<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

Sign in to RStudio

Username:
jon9348

Password:
.....

Stay signed in

Sign In

The screenshot shows the RStudio interface running on a web browser. The title bar indicates the URL is rstudio.questanalytics.northwestern.edu. The main window displays the R console output:

```
R version 3.6.3 (2020-02-29) -- "Holding the Winsorized"
Copyright (C) 2020 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)

R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

Natural language support but running in an English
locale

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help,
or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> |
```

The RStudio interface includes a sidebar with tabs for Environment, History, and Connections, and a bottom panel with tabs for Files, Plots, Packages, Help, and Viewer.

<https://jupyter.questanalytics.northwestern.edu>

Python 3.7.1

Sign in

Username:
jon9348

Password:
.....

Sign In

The screenshot shows a web-based Jupyter Notebook interface. At the top, there's a header bar with navigation icons, a URL bar showing the address, and user profile information. Below the header is a logo and a "Logout" button. The main area has tabs for "Files", "Running", and "Clusters", with "Files" currently selected. A message says "Select items to perform actions on them." There are buttons for "Upload", "New", and a refresh icon. The main content is a file browser listing several directories. The columns are "Name", "Last Modified", and "File size". The listed directories are:

Name	Last Modified	File size
archives	3 months ago	
bin	a day ago	
biobakery	3 years ago	
bioinformatics	2 years ago	
command	2 years ago	
conda-bld	3 months ago	
Desktop	3 years ago	
Downloads	2 years ago	
ebtest	4 years ago	
ftp-trace.ncbi.nlm.nih.gov	a year ago	
GATK	2 years ago	
globus	3 years ago	

High-Memory Nodes GPU Nodes

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

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Quest



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3	Quest FAQ	90865	2019-12-20	3040
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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

Quest: High Performance Compute Cluster

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

The screenshot shows the official website for Globus. The header includes a search bar, a star icon, and a user profile picture. The main navigation menu has links for 'I Want To...', 'Pricing', 'Resources', 'Support', 'About', and 'Log In'. A large banner in the center promotes 'GlobusWorld 2020' as a virtual event on April 29, 2020, with a link to visit globusworld.org for more information. Below the banner, the tagline 'Research data management simplified.' is displayed, along with three service icons: 'TRANSFER' (file icon), 'SHARE' (people icon), and 'BUILD' (hexagon icon).

globus
a uchicago non-profit service

I Want To... ▾

Pricing ▾

Resources ▾

Support ▾

About ▾

Log In

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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

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.

The screenshot shows the Globus File Manager interface. On the left is a sidebar with icons for FILE MANAGER, BOOKMARKS, ACTIVITY, ENDPOINTS, GROUPS, CONSOLE, ACCOUNT, LOGOUT, and HELP. The main area has two tabs at the top: "Northwestern Quest" and "JLocal". The "Northwestern Quest" tab is active, showing a path of "/~/". Below the tabs is a toolbar with "select all", up and down arrows, a refresh icon, and a gear icon. A modal window is open in the center, listing files from the left collection and actions for them. The files listed are:

File/Folder	Last Modified	Size
0.732201258492754.tmp	08/03/2018 12:47pm	26.46 MB
0105528.pdf	03/08/2018 04:16pm	684.35 KB
2019_users	04/12/2019 02:58pm	9.32 MB
7_10-7_11.txt	07/16/2019 08:11pm	967.35 KB
7_10-7_17.b1042.txt	07/16/2019 07:41pm	3.48 MB
7_10-7_17.b1042A.txt	07/16/2019 07:42pm	1.46 MB
7_11-7_12.txt	07/16/2019 08:13pm	1.47 MB
7_12-7_13.txt	07/16/2019 08:15pm	1.07 MB

The actions available for selection are:

- Share (with user icon)
- Transfer or Sync to... (with double arrow icon)
- New Folder (with folder icon)
- Rename (with edit icon)
- Delete Selected (with trash bin icon)
- Download (with cloud icon)
- Open (with document icon)
- Upload (with cloud icon)
- Get Link (with link icon)
- Show Hidden Items (with eye icon)
- Manage Activation (with power icon)

At the bottom of the interface are three buttons: "Start" (with play icon), "Transfer & Sync Options" (with dropdown arrow), and another "Start" button (with play icon).

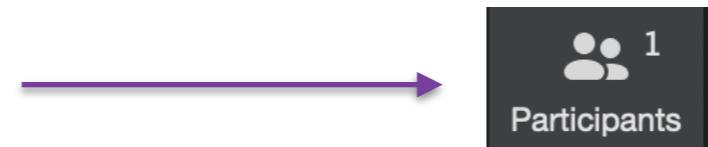
<https://app.globus.ora/activity>

BREAK

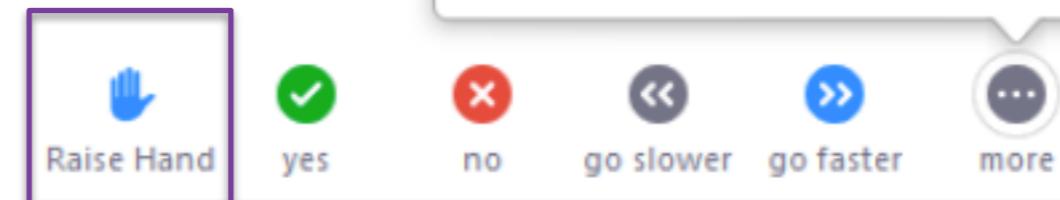
Please set up your screen to have Zoom on one half of the screen and a terminal or web browser on the other half.

“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?

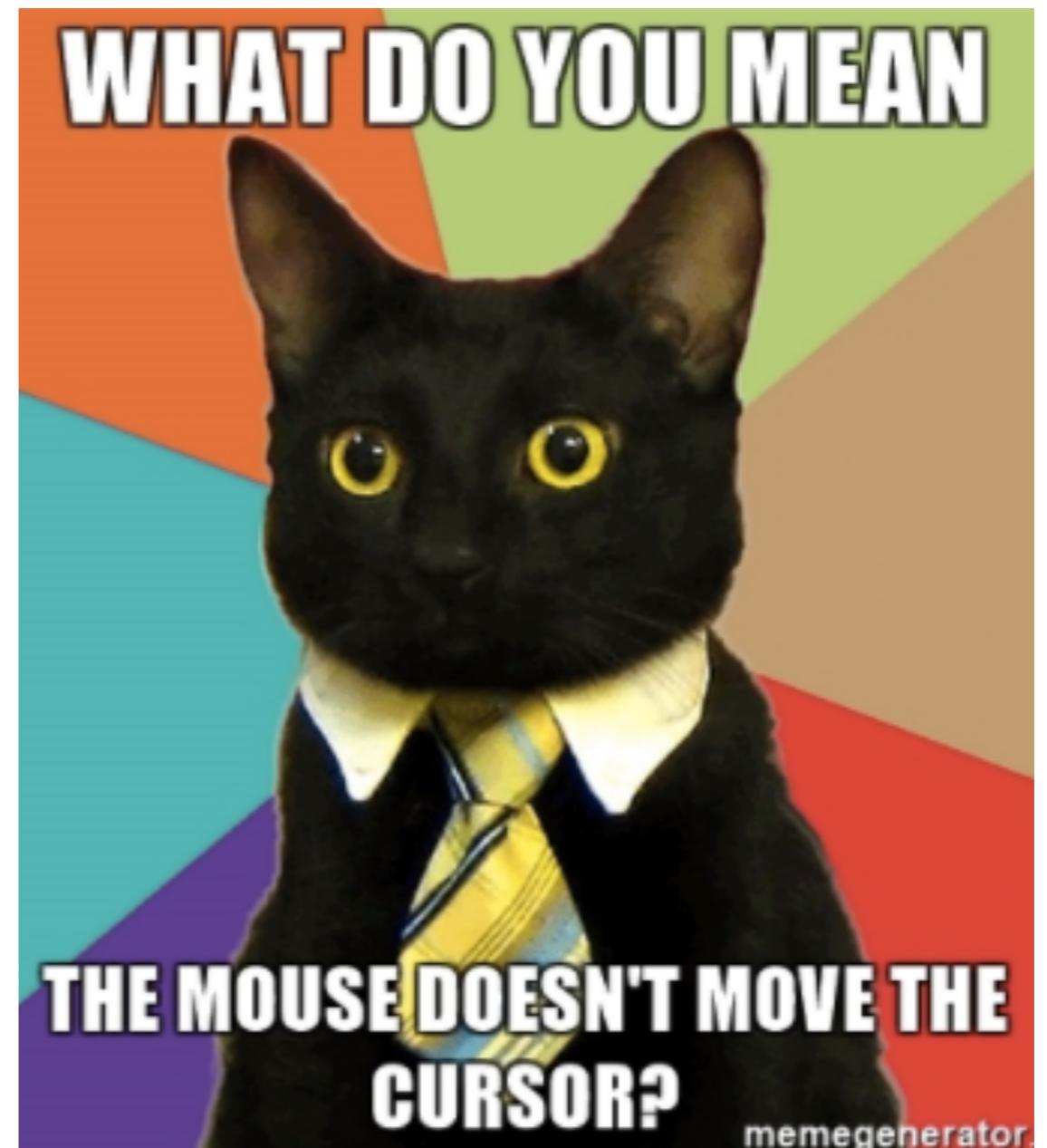
If your Allocation:

- 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 -xvzf 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

Run:

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

Linking to
libraries
&headers