Computational Skills for Researchers
Intro to Quest

Pascal Paschos, Sr. HPC Specialist
Research Computing Services

https://github.com/nuitrcs/intro_quest_workshop

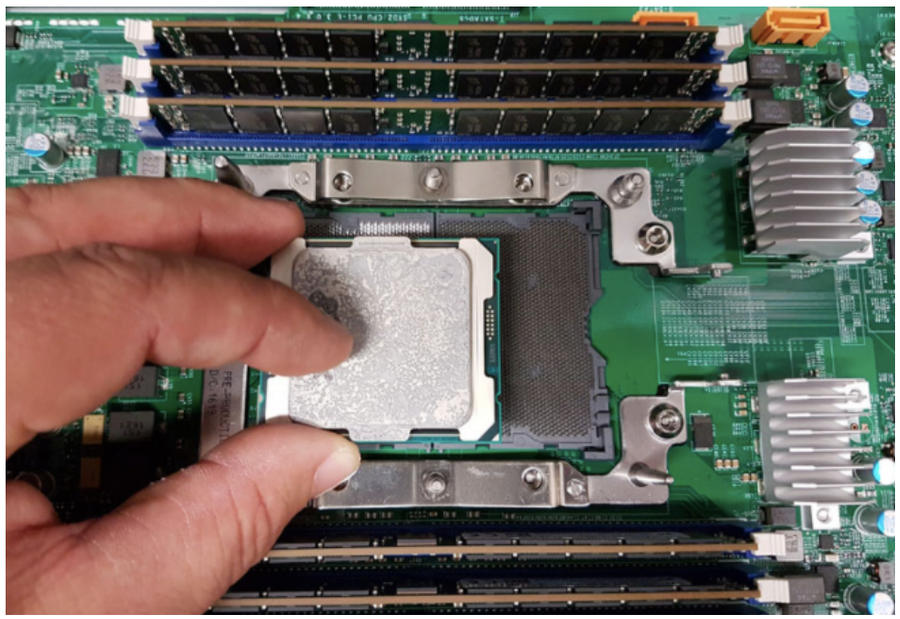
Northwestern
INFORMATION TECHNOLOGY

Quest: High Performance Computing Cluster

“node”: a computer

>800

56 GPUs



“core”: a processor

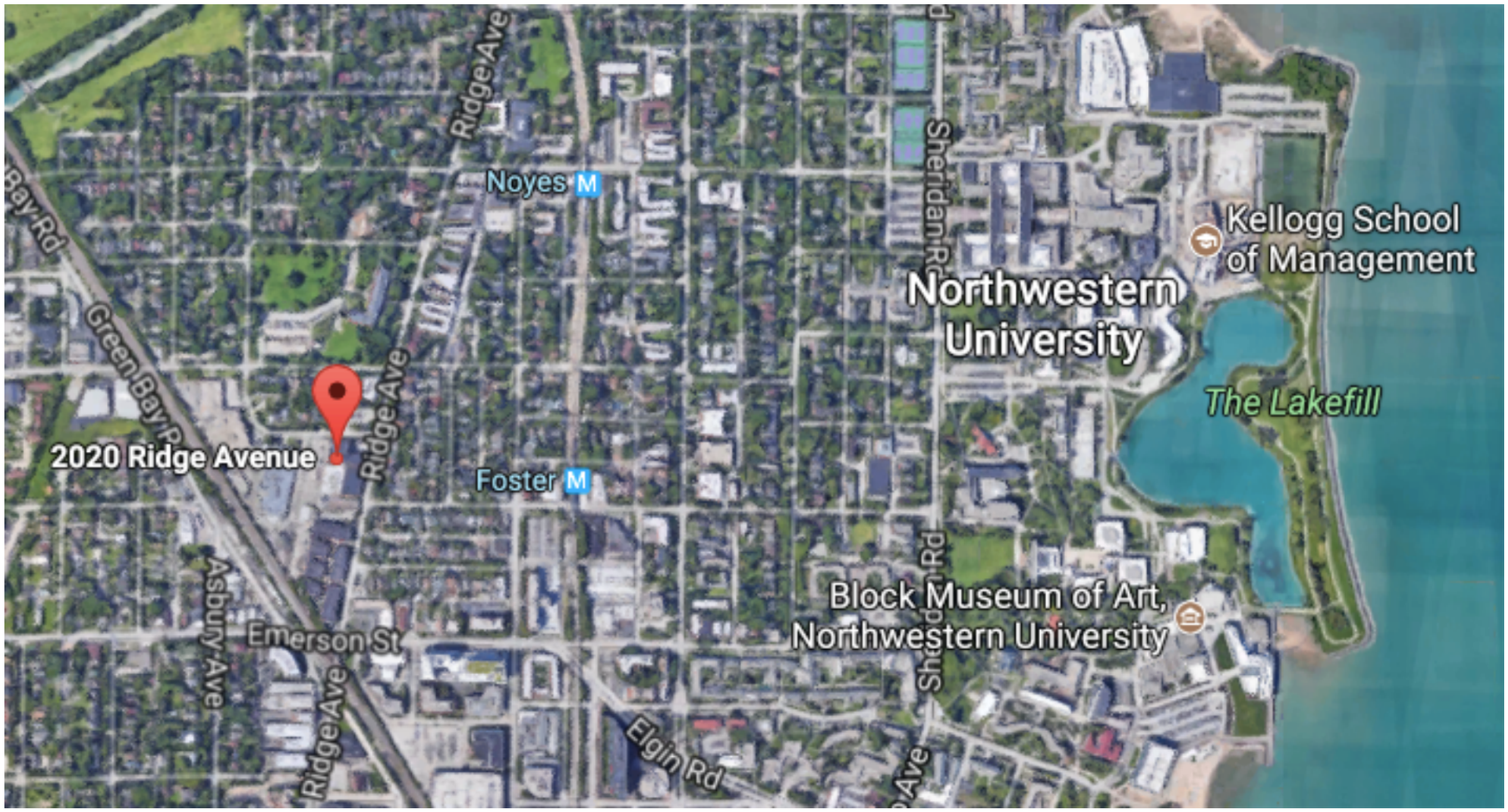
~20,000

Quest: High Performance Computing Cluster

"infiniband": high-speed inter-connect

nodes in racks

Quest: High Performance Computing Cluster



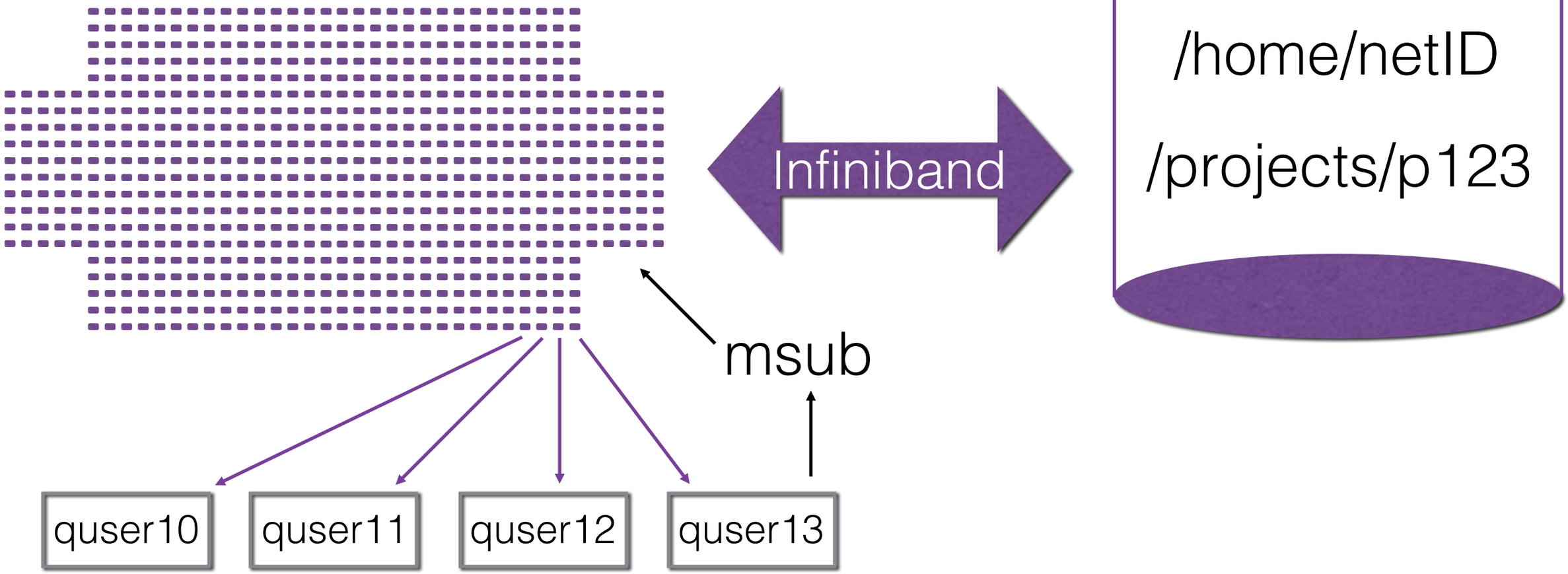
24 hour on-site security, 3-factor authentication, firewalls and intrusion detection systems, dedicated power station, high-throughput network

Quest: High Performance Compute Cluster

Allocation: compute hours, storage space, group

800 compute nodes

128 GB RAM



login nodes

ssh netID@quest.northwestern.edu

Analytics Nodes

The Quest Analytics Nodes allow users to run RStudio 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.

Backing up your data

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

RDSS & FSMRESfiles

Amazon AWS

Parallel Computing

Multiple jobs working independently

"embarrassingly parallel"

"pleasingly parallel"

high-throughput computing

Single job communicating across nodes

message passing:

MPI, OpenMP

Software

https://kb.northwestern.edu/quest-software

Quest: Logging in and Getting started

Mac users: launch the Terminal App:

ssh <netID>@quest.it.northwestern.edu

PC users: launch PuTTY (preferred) or FastX:

Hostname : quest.it.northwestern.edu

Username : your Northwestern NetID

Password : your Northwestern NetID password

Quest: Logging in and Getting started

1) login to Quest
   `$ssh` quest.northwestern.edu

2) where are you?
   `$pwd` -> this is your home directory

3) what is the name of your project allocation?
   `$groups` (your project is in **`/projects/<allocation>`**)

4) what is the status of your project?
   `$checkproject <allocation>`

5) how much space is used in your home dir?
   `$homedu`

Quest: Logging in and Getting started

1) login to Quest
   `$ssh` quest.northwestern.edu

2) where are you?
   `$pwd` -> this is your home directory

3) what is the name of your project allocation?
   `$groups` (your project is in **`/projects/<allocation>`**)

4) what is the status of your project?
   `$checkproject <allocation>`

5) how much space is used in your home dir?
   `$homedu`

Quest: Logging in and Getting started cont

6) Check status of cluster jobs: **`$ showq -r`**

7) Check load on the login node: **`$ top`**

8) Check modules: **`$ module avail`**

9) Load a browser: **`$ module load firefox ; firefox`**

10)Load a python **`$ module load python ; python`**

11)Load a MATLAB
`$ module load matlab/r2016a ; matlab`

Quest: Getting started with Cyberduck

To connect to Quest, start Cyberduck and then :

1) **Click Open Connection** in the upper left of the Cyberduck window At the top of the Open Connection window that appears, Select SFTP (SSH File Transfer Protocol) from the drop-down menu.

2) **Enter quest.it.northwestern.edu** for server specification

3) **Enter your NetID** in the Username: box and leave the Password: box empty to prevent your NetID password from being saved in a file on your personal computer. Public Key Authentication is not supported.

4) **Click Connect**. You will see a Login failed window.

5) **Enter your NetID password** in the Password: field.

6) **Click Login.**

Quest: transfer intro.tar with Cyberduck

<u>On your local machine</u>
locate your intro.tar file in your Downloads directory

Drag intro.tar into your home directory in Cyberduck

<u>On the command line window that's logged into Quest</u>
$ ls confirm intro.tar is in the directory that you are in

$ tar -xvf intro.tar to unpack the tar file

$ ls look for the unpacked files "submit_generic.sh" and "helloworld.py"

$ cat submit_generic.sh take a look at the header of this file

Quest: transfer intro.tar with git

On the command line window that's logged into Quest

$ git clone https://github.com/nuitrcs/intro_quest_workshop

$ cd intro_quest_workshop

$ tar -xvmf intro.tar to unpack the tar file

$ ls look for the unpacked files "submit_generic.sh" and "helloworld.py"

$ cat submit_generic.sh take a look at the header of this file

Quest: submit_generic.sh

```
#!/bin/bash
#MSUB -A <allocationID> ## <-- EDIT THIS TO BE YOUR ALLOCATION
#MSUB -q <queue_type>   ## <-- EDIT THIS TO BE YOUR QUEUE NAME
#MSUB -l nodes=1:ppn=1
#MSUB -l walltime=00:10:00
#MSUB -N sample_job
#MSUB -o outlog
#MSUB -e errlog

cd $PBS_O_WORKDIR       ## the directory from which the job was
submitted
module load python      ## Load necessary modules (software pr
libraries)

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

Quest: submitting a job

login node

"msub submit.sh"

scheduler

```
#MSUB -A <allocationID>
#MSUB -q <queue_type>
#MSUB -l nodes=1:ppn=1
#MSUB -l walltime=00:10:00
```

compute node

compute node

compute node

compute node

compute node

Quest: sample bash submission script

What is the scheduler looking for in your script?

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

Account: `#MSUB -A p20XXX`

Queue: `#MSUB -q short`

Number of nodes & cores: `#MSUB -l nodes=1:ppn=1`

Length of the job: `#MSUB -l walltime=00:10:00`

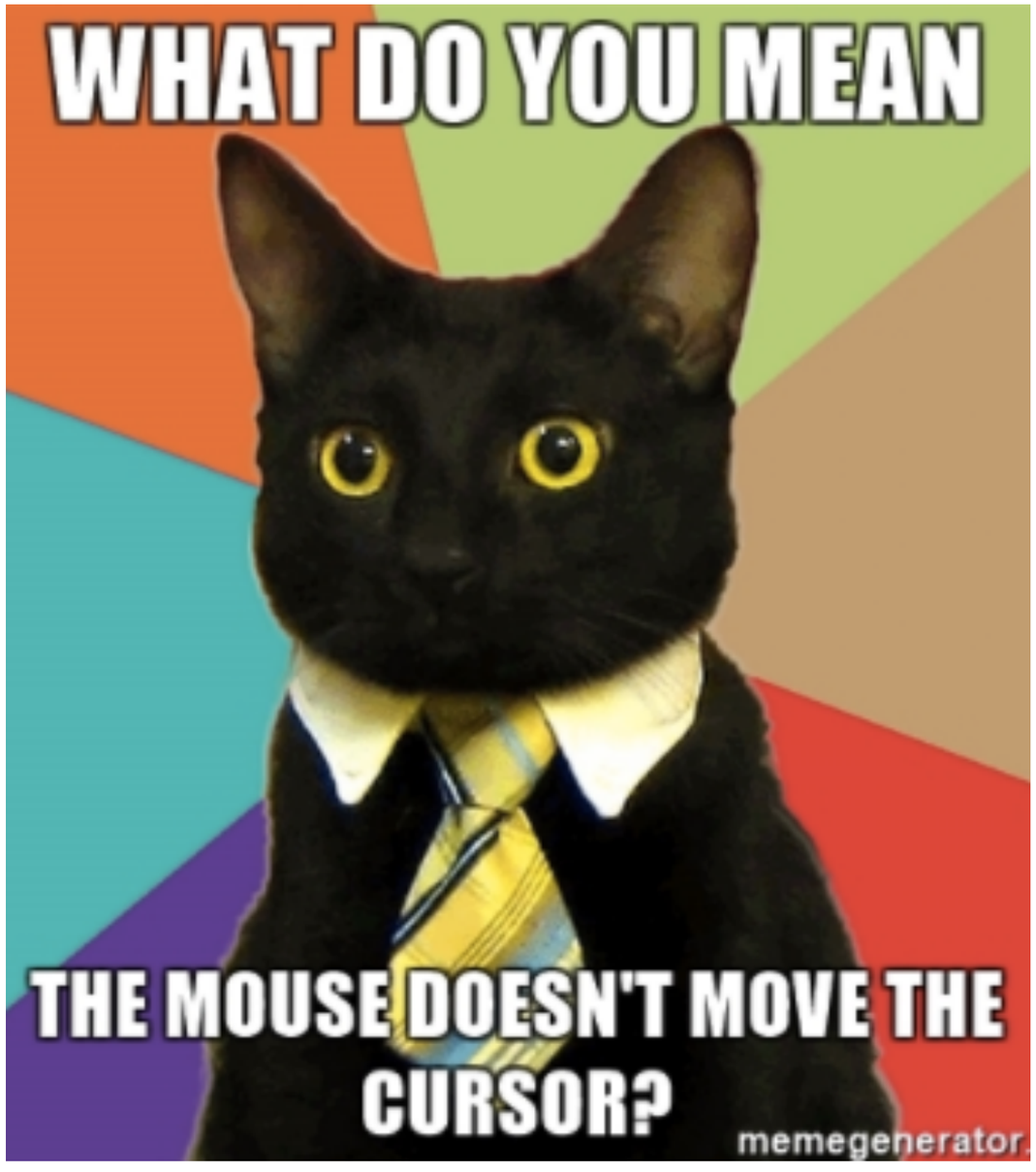
Name the job: `#MSUB -N sample_job`

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

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

text editor: vi/vim

- **On command line: “vi submit_generic.sh”**
- **You land in command mode**
- **To enter insert mode: “i” where the cursor is; “o” inserts one line below that**
- **Navigate with arrow keys**
- **To exit insert mode: “esc”**
- **To save: “:w”**
- **To exit: “:q”**
- **To exit without saving: “q!”**



Quest: sample bash submission script

1) submit your job

```
$msub submit_generic.sh
```

2) copy the job_id msub returns

3) where is your job in the queue?

```
$showq -u <your netID>
```

4) what is the status of your job?

```
$checkjob <job_id>
```

Jobs on Quest

https://kb.northwestern.edu/page.php?id=69247

Example Jobs

https://kb.northwestern.edu/page.php?id=70719

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 env 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$HOME/fftw_install/lib -lfftw3 -lm **
  -I$HOME/fftw_install/include
- Run:
  - **./test >& output**

Compiler-Source-Exec

Linking to libraries &headers

Questions?

email: quest-help@northwestern.edu

Research Computing Services

Northwestern
INFORMATION TECHNOLOGY