UNIVERSITY of CALIFORNIA · IRVINE

Intro to Linux on the HPC cluster

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Some talking points..

- You've heard of Linux...? (~ Darwin/BSD, very unlike Windows, but .. Cygwin!)
- You're interested & bright
- You can Google, and read further by yourself.
- Questions, ASK THEM, but I may not answer them immediately. – "*You don't know what you don't know*"

Computing Philosophy

- Unlike your Science...
- Be lazy.
- Copy others.
- Don't invent anything you don't have to.
- Re-USE, re-CYCLE, DON'T re-invent.
- Don't be afraid to ask others.
- Resort to new code only when absolutely necessary.

Philosophy – Take Away

- You're not CS, not programmers
- Don't try to be them
- But! Try to think like them, at least a bit
- Google is your friend

Getting Help

- Fix IT Yourself with Google <goo.gl/05MnTi>
- Listservs, forums, IRCs are VERY useful for more involved questions.
- The HPC Web page http://hpc.oit.uci.edu/ and HOWTOs there.
- Us – Harry, Garr, Joseph, Edward
- BUT!! Unless you ask questions intelligently, you will get nothing but grief.

How to Ask Questions

- Reverse the situation: if you were answering the question, what information would you need?
- Not Science, but it is Logic.
- Include enough info to recreate the problem.
- Exclude what's not helpful or ginormous (use <pastie.org> or <tny.cz>)
- Use text, not screenshots if possible.

Bad Question

Why doesn't "X" work?

Good Question

I tried running the new podunk/2.8.3 module this morning and it looks like I can't get it to launch on the Free64 queue. My output files aren't helping me figure out what is wrong.

I am working out of /bio/joeuser/RNA_Seq_Data/
and the qsub script is 'job12.sh'. The output should be in /bio/joeuser/RNA_Seq_Data/output.

I tested it in my login shell with a small data set and it worked OK, but when I submit the job, it appears to go thru the scheduler but then dies immediately when it hits the execution node.

I can't find any output to tell me what's wrong, but the error messages suggest that there's a problem finding libgorp.so.3

HELP US HELP YOU

We Need:

- the directory in which you're working (*pwd*),
- the machine you're working on (*hostname*)
- modules loaded (*module list*)
- computer / OS you're connecting from
- the command you used and the error it caused (in /text/, not screenshot)
- much of this info is shown by your prompt

see <http://goo.gl/6eZORd>

On to HPC

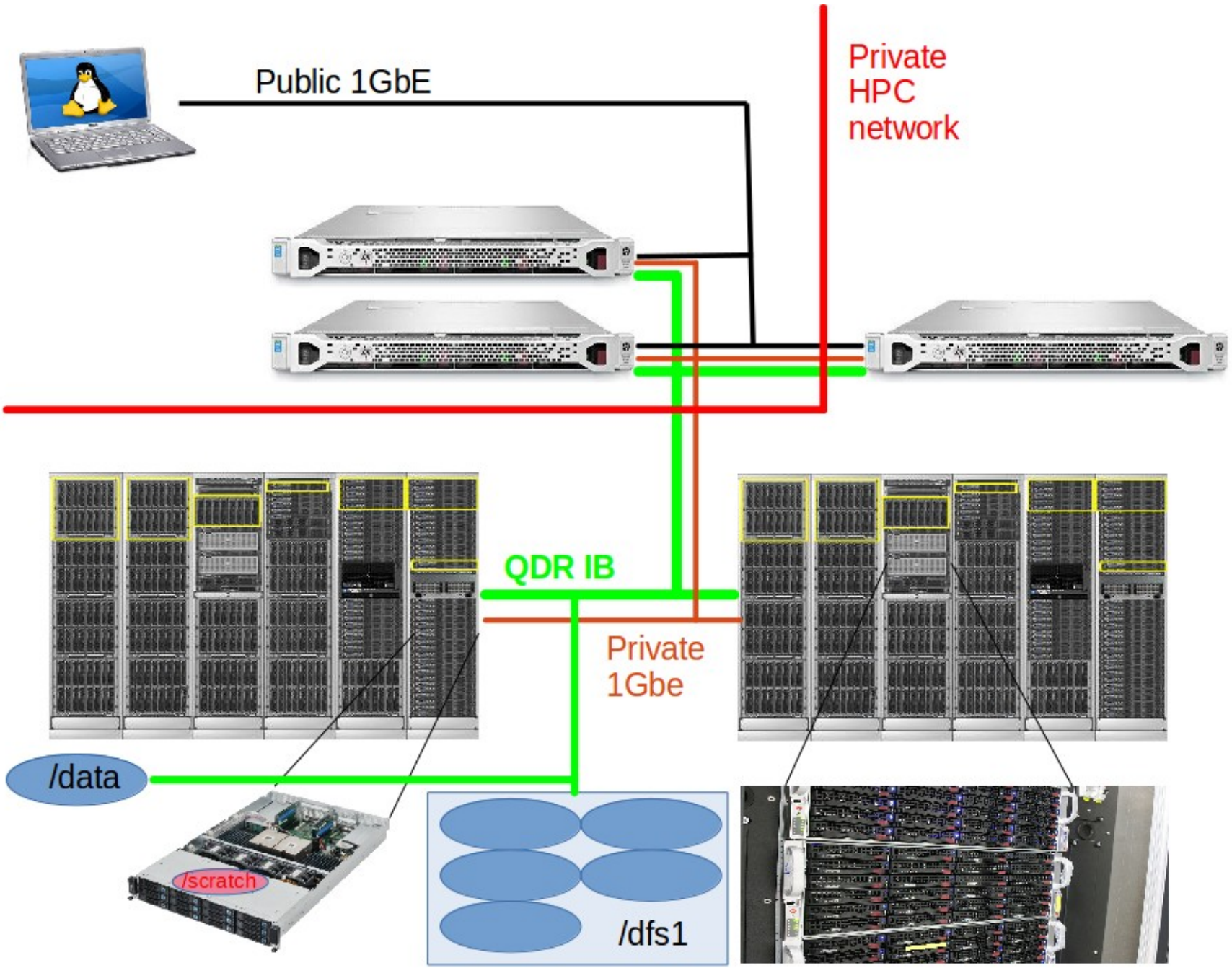
What is the H$_{igh}$ P$_{erformance}$ C$_{omputing}$ Cluster?

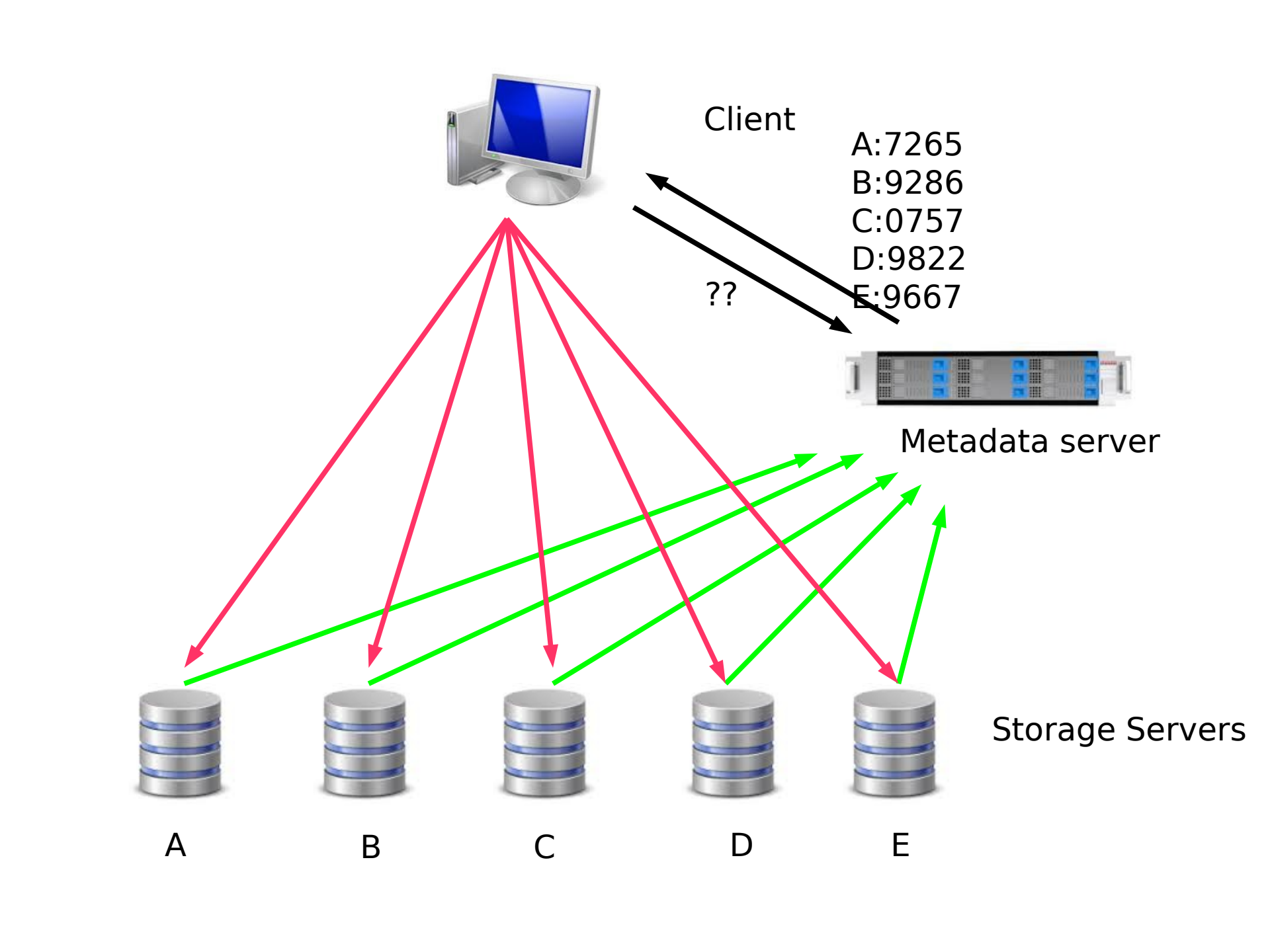
and…

Why do I need HPC?

What is a Cluster?

- Pod of large general purpose computers
- run the Linux Operating System
- linked by some form of networking
- have access to networked storage
- can work in concert to address large problems
- by scheduling jobs very efficiently


Public 1GbE
Private
HPC
network
QDR IB
Private
1Gbe
/data
/scratch
/dfs1


Client
A:7265
B:9286
C:0757
D:9822
E:9667
??
Metadata server
Storage Servers
A
B
C
D
E

What HPC is

- ~7400 64b Cores – Mostly AMD, few Intel
- ~44TB aggregate RAM
- ~1.3PB of storage
- Connected by 1Gb ethernet (100MB/s)
- Connected by QDR IB (4000MB/s)
- Grid Engine Scheduler to handle Queues
- > 1950 users, 100+ are online at anytime

What HPC is NOT

- NOT: your personal machine
- It is a shared resource.
- What you do affects all the other users, so think before you hit that 'Enter' key.
- Well secured from mischief and disasters – not an invitation

DATA IS NOT BACKED UP

- NO DATA IS BACKED UP – WHAT. SO. EVER. -- Lobby your PIs to get us more $ if you want this.
- Most data is stored on RAID6
- BUT! Any of that can disappear at any moment. It has.
- IF IT'S VALUABLE, back it up elsewhere --- or the code that generated it.

Backup Possibilities

- Your UCI 'Google Drive' can be connected to HPC to back up small files

- You can buy a USB drive to use as a backup →

- Use '**rsync**' to do incremental backups to it:

```
rsync -av this_dir MyMac:/this_dir
```

- Your lab can buy a NAS device and mount it on HPC as an NFS mount

- Your lab can rent space on another filesystem.

HPC FileSystem Layout

Orange – Cluster Wide
Black – Node Specific

/

├── data/	NFS Mount		
|─apps	All Programs are installed here		
+─users	Users home directory	– 50GB LIMIT PER USER	
|----- pub/	Public scratch space, overflow	- 2 TB limit (but only active data)	
├── bio/	Space for BIO group → /dfs1		
├── som/	Space for SOM group → /dfs1		
├── cbcl/	Space for CBCL group → /dfs1		
├── dfs1/	BeeGFS Distributed File System	~460TB	
|----- dfs2/	BeeGFS Distributed File System	~190TB	
├── scratch	Node-specific temporary storage per job (faster than all above)		~1TB – 14TB
├── fast-scratch	High Speed Fraunhofer FileSystem for temporary storage		- 13TB
|----- ssd-scratch	Very High IOPS for DB, other jobs.		
├── /tmp	Same as scratch		

Disk Space / Quotes / Policies

- You can only have so much space
- 50GB for /data/ (home directory)
- if 6months or older without use – please remove from cluster
- More for Condo owners or Groups who have bought extra disk space.
- Regardless, NO DATA IS BACKED UP

Data Sizes

- Your data will be BIG – “BigData”
- BigData is somewhat 'dangerous' due to its bigness.
- Think before you start. You can't predict everything, but you can predict a lot of things – more on this later

Network Considerations

From Cox.net ↔ UCI

```
$ traceroute moo.nac.uci.edu
traceroute to moo.nac.uci.edu (128.200.34.95), 30 hops max, 60 byte packets
 1  haggis.net (192.168.1.1)  0.694 ms  0.940 ms  1.134 ms
 2  172.27.35.1 (172.27.35.1)  2.232 ms  2.301 ms  2.394 ms
 3  10.75.151.1 (10.75.151.1)  11.647 ms  11.766 ms  11.855 ms
 4  ip68-4-13-176.oc.oc.cox.net (68.4.13.176)  12.249 ms  16.099 ms  16.845 ms
 5  ip68-4-11-12.oc.oc.cox.net (68.4.11.12)  17.661 ms  18.192 ms  18.181 ms
 6  68.1.1.171 (68.1.1.171)  18.989 ms  23.355 ms  13.053 ms
 7  xe-5-1-1.edge2.LosAngeles9.Level3.net (4.53.230.93)  16.391 ms xe-5-0-
1.edge2.LosAngeles9.Level3.net (4.53.230.85)  16.392 ms xe-9-0-
1.edge2.LosAngeles9.Level3.net (4.53.230.229)  17.202 ms
 8  * * *
 9  CENIC.ear1.LosAngeles1.Level3.net (4.35.156.66)  20.376 ms  20.806 ms  20.817 ms
10  dc-uci-uci1--dc-lax-agg6-egm.cenic.net (137.164.24.42)  23.856 ms  24.259 ms  24.261 m
11  cpl-core--cs1-core-kazad-dum-hsrp.ucinet.uci.edu (128.200.2.194)  20.705 ms  20.684 ms
20.660 ms
12  msd-core--cpl-core.ucinet.uci.edu (128.195.248.250)  18.776 ms  18.656 ms  18.152 ms
13  415--msd-core.ucinet.uci.edu (128.195.250.162)  19.409 ms  19.281 ms  19.523 ms
14  moo.nac.uci.edu (128.200.34.95)  19.151 ms  19.084 ms *
```

Network Considerations

Inside UCI (moo ↔ HPC)

```
$ traceroute hpc.oit.uci.edu
traceroute to hpc.oit.uci.edu (128.200.84.34), 30 hops max, 60 byte packets
 1  415-vl110.ucinet.uci.edu (128.200.34.1)  0.434 ms  0.524 ms  0.586 ms
 2  cs1-core--415.ucinet.uci.edu (128.195.249.233)  0.376 ms  0.380 ms  0.416 ms
 3  dca--cs1-core.ucinet.uci.edu (128.195.239.182)  0.488 ms  0.594 ms  0.736 ms
 4  hpc-login-4.oit.uci.edu (128.200.84.34)  0.313 ms  0.300 ms  0.283 ms
```

How to: Login with SSH

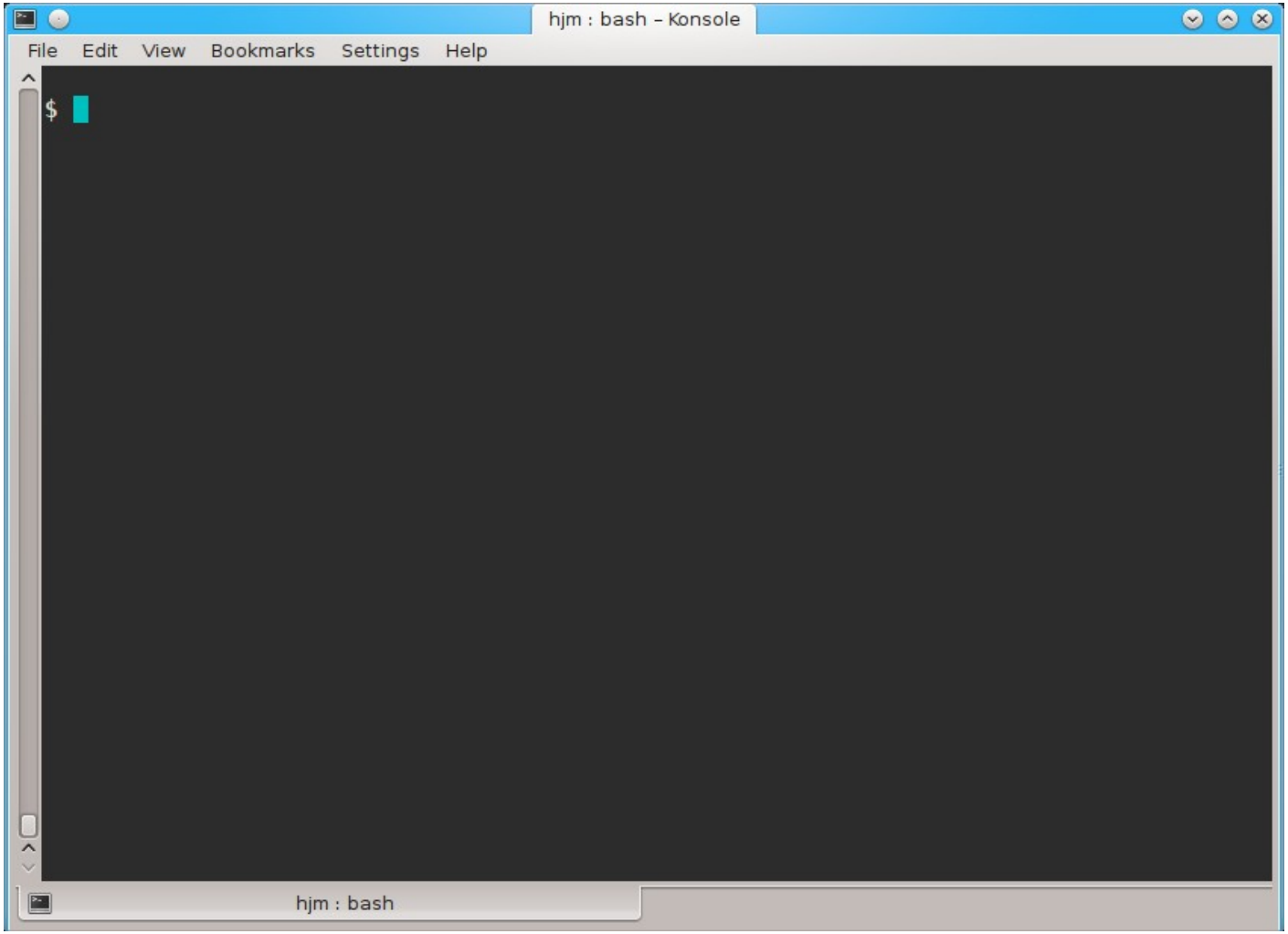
- SSH is an encrypted protocol so that info over the connection can't be deciphered by others.
- You MUST use SSH to connect to HPC, using the ***command line....***

- Underlies 'scp' (secure copy), sftp
- Also 'sshfs' which allows you to attach your filesystem to HPC (or vice versa).

Here vs There

- Your laptop is HERE (and HERE is often dynamic)
- (How do you find out your IP #?)
- HPC is THERE (and THERE is always static)
- Files have to get from HERE to THERE (so it's always easier to push data from HERE to THERE, but …..)
- Displays are generated THERE but are seen HERE. (both Text and Graphics).
- The point above can be exploited to make life easier. [byobu and x2go]
- Make sure of where you are and in which direction the bytes are going.

Commandline Hell



Command Line Cons

- The tyranny of the blank page
- No visual clues
- Type vs click
- Have to know what to type
- HOW DO YOU KNOW WHAT TO TYPE???

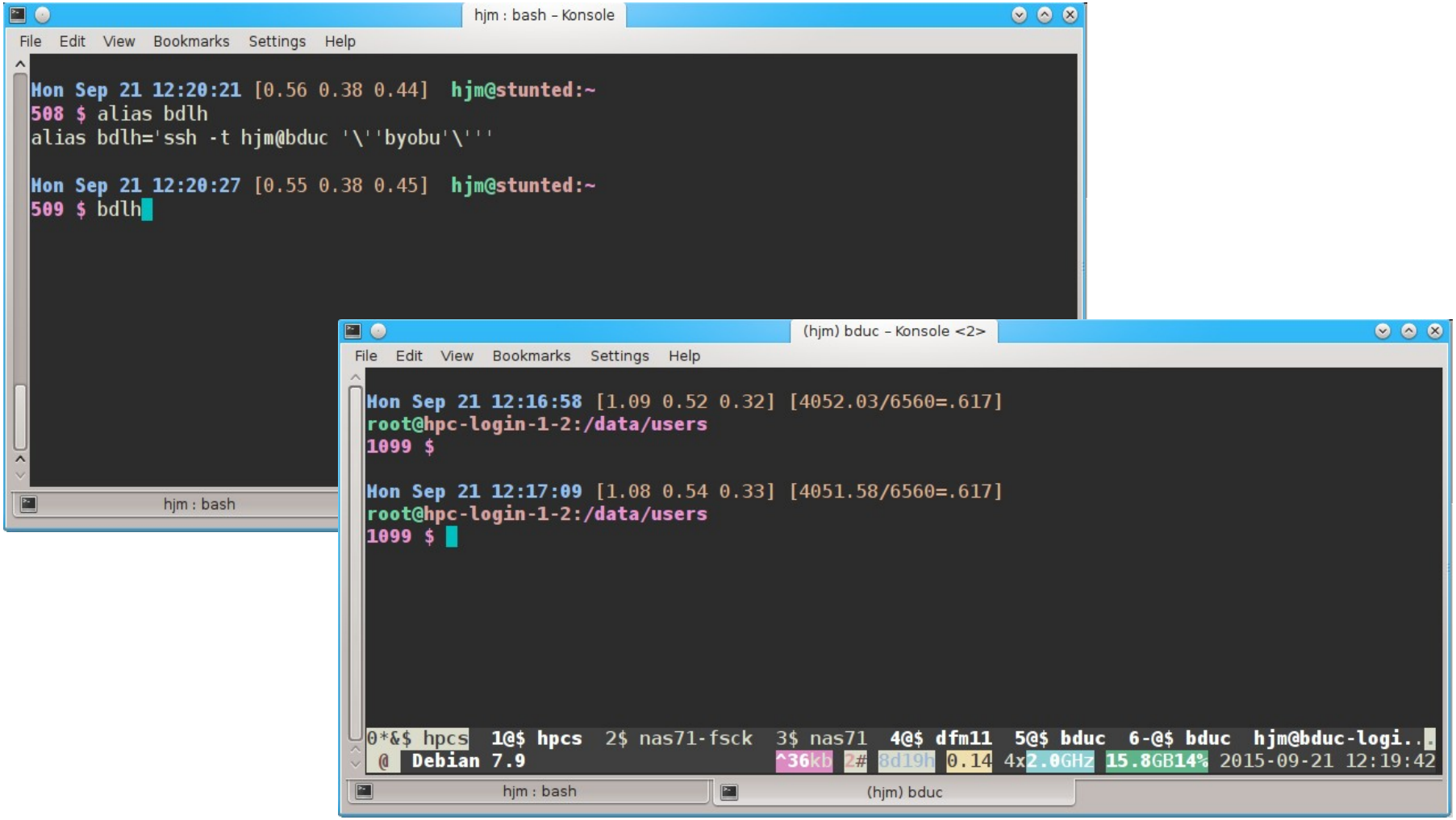
Command Line Pros

- It doesn't get much worse than this
- When you do learn it, you'll know it and it probably won't change for the rest of your life
- It's a very efficient way of interacting with the computer (which is why it's survived for 50+yrs).
- You can use it to create simple, but very effective pipelines and workflows.

Keeping SSH Session Alive

- If you need to maintain a live connection for some reason, use 'byobu or screen'.
- It allows you to multiplex and maintain connections in a single terminal window.
- Somewhat unintuitive interface but very powerful.
- You know about ***cheatsheets*** (Google!!)

Byobu / Screen



Graphics Apps on HPC

- Linux uses X11 for graphics
- X11 is very chatty, high bandwidth, sensitive to network hops/latency.
- If you need graphics programs on HPC, use x2go vs native X11, which does for graphics what byobu does for terminal screens.
- x2go is described in the Tutorial & HOWTO, also GOOGLE

How to: SSH & The Shell

- Once logged in to HPC via SSH you are now using the *Shell,* which is..
- A program that intercepts and translates what you type, to tell the computer what to do.
- What you will be interacting with mostly.
- HPC shell is '***bash***', altho there are others.

Learn the shell, or else.

- If you don't get along with the shell, life will be hard.
- Before you submit anything to the cluster via qsub, get it going in your login shell.
- You're welcome to start jobs in on the IO node, type: `qrsh`
- "*DO NOT RUN JOBS ON THE LOGIN NODE*"

How to know if I am on Login Node?

Look at your shell prompt!

- Mon Mar 28 21:05:29 [0.02 0.18 0.23] user@hpc-login-1-2:~
  1 $

- Can also use the command **`hostname`**

  Mon Mar 28 21:05:29 [0.02 0.18 0.23] user@hpc-login-1-2:~
  1 $ **hostname**
  hpc-login-1-2.local

Command Line Editing

- Since you'll be spending a lot of time fighting with the cmd line, make it easy on yourself.
- Learn cmd line editing to edit previous cmds
- Up/Down arrow keys scroll thru cmd history
- L/R arrow keys scroll by 1 char
- `^` means CONTROL Key
- `^` makes L/R arrow jump by a word (usually)
- Home, End, Insert, Delete keys work (except Macs lack 'Delete' keys (because … Steve Jobs)
- `^u` kills from cursor left; `^k` kills from cursor to right
- Tab for auto complete

STDIN, STDOUT, STDERR

- ***T H I S I S I M P O R T A N T***
- STDIN is usually the keyboard, but...
- STDOUT is usually the screen, but...
- STDERR is *also* usually the screen, but...
- All can be redirected all over the place
- to files, to pipes, to FIFOs to network sockets
- can be combined, split (by 'tee'), to make simple workflows
- More on this later.

File & Directories

- Files & Directories much like on Mac & Win
- Except...
- Names are case-sensitive, 256 char long
- 'Folders' → 'Directories' , separated by '/'
- No spaces in names*
- . means 'in this dir’
- .. means parent dir
- ~ means 'home dir'
- A leading '/' means 'from the root dir'

Foreground & Background Jobs

- Foreground (**fg**) jobs are connected to the terminal. You kill a **fg** job with **^C**.
- Background (**bg**) jobs have been disconnected from the terminal and are running in the **bg**.
- Send a job to the **bg** immed. by appending **&**
- Recall a job to the **fg** with **fg**.
- Send a **fg** job to the **bg** with **^z** (suspend), then '**bg**'.
- All jobs started in the terminal are killed when you log out. (usually)

Pipe |

- Works with STDIN/OUT/ERR to create 'pipelines'
- Very similar to plumbing; can add '**tee**'s to introduce splits.

```
$ ls | tee 1file 2file 3file | wc
```

- STDOUT of one program goes to the STDIN of another command whose STDOUT goes to the STDIN of another program ad infinitum.
- Sooooo.....

Pipe Example

```
w|cut -f1 -d' '|egrep -v "(^$|USER)"|sort|uniq -c|wc
```

w spits out who is on the system right now

cut -f1 -d ' ' chops out the 1st field (the user), based on the space token

egrep -v "(^$|USER)" filters out both blank lines and lines with 'USER'

sort sorts the usernames alphabetically

uniq -c counts the unique lines

wc -l word-counts that output.

Example: Now on HPC!

Help on Commands

- **`cmd -h`**
- **`cmd -help`** `or` **`cmd --help`**
- **`man cmd`**
- **`info cmd`** (but you hope not)
- And ….. Google...

Some Useful Commands

- ls [many options] = list fil<tab><tab>
- cd [up or down] = change directory
- find [from] -name [name] = find files
- locate [name] = where is this file?
- tree [options] = show the dir tree
- file [name(s)] = what is this?
- du = disk usage
- df = disk free
- less [names] = view files
- cols [file] = view file in columns

Creative / Destructive Commands

- mkdir [name] – make a dir
- rmdir [name] – remove a dir
- mv [from] [to] = move or rename
- cp [from] [to] = copy file(s)
- rm [file] = delete file(s)
- wget [URL] = get a file from the Internet
- curl -O [URL] = ditto, but on steroids

More Useful Commands

- mc = Midnight Commander
- [ah]top = top CPU-using processes
- time [command] = how long does it take?
- [aef]grep [regex] [files] = find regex in files
- cat [files] = print the files to STDOUT
- head/tail [files] = dump the top / bottom of files

Regular Expressions

- Among the most powerful concepts in pattern matching
- Simple in concept, NASTY in implementation
- Among the ugliest / most confusing things to learn well
- But pretty easy to learn the simple parts.
- You will NEED to learn it – it's central to computers and especially biology

Regexes

- Simplest form is called globbing: **a***
- Barely more complicated : **a*.txt**
- A bit more: **a*th.txt**
- Can be MUCH more complex:
- **[aeiou]** = any of 'aeiou'
- **F{3,5}** = 3-5 'F's
- **H+** = 1 or more 'H's
- . = any character
- Also classes of characters (#s, alphabetic, words)

Archiving / Compression

- tar = std archive format for Linux
- zip = common archive format, from Windows
- gzip/unzip = common compressed format
- bzip2/bunzip2 = another compressed format
- pigz = parallel gzip (for large files)
- pbzip – parallel bzip2 (ditto)

Customize Your Environment

- Set aliases (`alias nu="ls -lt |head -22"`)
- Set Environment Variables (`export EDITOR=vim`)
- Change your bash behavior via ***shopt***
  (google for how)
- Make these permanent via `.bash_profile` & `.bashrc` files in your *home directory*

Editing Files: simple & complex

- Text-based:

•nano, joe, vi/vim, emacs

- GUI-based:

•gedit, nedit, kate, jedit, emacs

(choose one and learn it, *well*)

Move Data to / from HPC

- Covered in detail in HPC USER HOWTO, which references: goo.gl/XKFEp
- scp, bbcp, netcat/tar on Mac, Linux.
- WinSCP, Filezilla, CyberDuck,FDT on Win
- Everyone should know how to use rsync. Not the easiest to learn, but very powerful & scriptable.
- rsync GUIs for Linux, Windows, MacOSX

Using Software on HPC

- 3 main sets of programs

- Your personal set (typically in ~/bin)

- The default system utilities

  cut, grep, ls, mv, cp, rm, cd, etc…

- The module system programs

The Module System

- **`[module avail]`** shows all installed software
- **`[module load R/3.01]`** loads program R version 3.01 (but doesn't start it)
- **`[module unload]`** unloads the specified program
- **`[module purge]`** removes all loaded programs
- **`[module list]`** lists all the currently loaded ones

How to Find Software

- locate <partial search term>
- apropos <search term>
- na<tab><tab> → name
- yum search <search term> # CentOS
- module avail (will dump all modules)
- Google
- Ask us.

The Scheduler (GE)

- Just another program that juggles requests for resources
- Make sure a program is working on a small set of test data on an interactive shell.
- Need a short bash script (aka ***qsub script***) to tell the GE what your program needs to run.
- Can improve the performance of your program in a variety of ways (staging data, running in parallel, using array jobs, etc)

The Scheduler: qsub vs qrsh

- *qrsh* will log you into an Interactive Node (IO Node) where you can test out your scripts

- IO Nodes are useful for GUI programs (X11 & x2go needed) or testing / running SMALL and FAST data sets

- *A qsub* script is just a series of bash commands that sets up your resource requirements, PATHs, executes your jobs, and does the post-processing. – NO USER INVOLVEMENTENT during the process

GE Useful Commands

- qstat - Queue Status
- queue / q – What queues you have access to
- qdel – Delete/Stop your job
- qhost – Show all nodes and their status

- Use `man cmd` to find out more information on above
- http://hpc.oit.uci.edu/PHPQstat

- Ref:
- http://hpc.oit.uci.edu/running-jobs
- http://hpc.oit.uci.edu/PHPQstat/

Sample QSUB Script

- Visit:
- <http://hpc.oit.uci.edu/guides/qsub-biolinux.html>

- Ref:
- <http://goo.gl/hrcXBg>

GE – Request Node Resources

- Use Case: You know your program requires at least
  24GB Memory
  16 CPU Cores
  You need to tell the scheduler

```
#$ -l mem_free=24G
#$ -pe openmp 16
```

This does not make your program run faster or use all cores – you simply reserve this amount

GE – Queues

- As you noticed, the scheduler uses queues to handle your job.
- Some queues have higher priority than others.
- Type **`queue`** or **`q`** to see what you have access to
- You specify these Qs in your qsub script with:

```
#$ -q som,free*
```

GE – Free and All Queue

- The free* queue allows anyone to use CPU cycles when they are not in use on any queue/node cluster wide

•When owners want to use their nodes, free* jobs are suspended

- Similar to the free* queue, the 'all' queue is group-specific: abio, asom, etc.

Big Data

- Volume

•Scary sizes, and getting bigger

- Velocity

•Special approaches to speed analysis

- Variety

•Domain-specific standards (HDF5/netCDF, bam/sam, FITS), but often aggregations of unstructured data

- BigData Hints for Newbies
  <http://goo.gl/aPj4az>

Big Data – How Big is Big?

# Bytes	Byte name / Abbriev'n	Approximation
1/8	bit (b)	0 or 1: the smallest amount of information.
1	Byte (B)	8 bits, the smallest chunk normally represented in a programming language.
2^{10}	1,024 B (1 KB)	a short email is a few KBs
2^{20}	1,048,576 B (1 MB)	a PhD Thesis ; Human Chr 1 is ~250 MB
2^{30}	1,073,741,824 B (1 GB)	the Human Genome is 3,095,693,981 B (optimized, ~780 Mb @ 2b/base) ; a BluRay DVD holds 25GB per layer (most movie BluRays are dual-layer = 50GB); a Genomic bam file is ~150GB
2^{32}	4,294,967,296 (4GB)	**fuzzy border between SmallData (32b) and BigData (64b)**
2^{40}	1,099,511,627,776 B (1 TB)	1/10th Library of Congress (LoC); the primary data fr. an Illumina HiSeq2K is ~5 TB
2^{50}	1,125,899,906,842,624 B (1 PB)	100X LoC; ~HPC's aggregate storage; ~100 PB is the yearly storage requirements of YouTube.
2^{60}	1,152,921,504,606,846,976 B (1 EB)	the est. capacity of the NSA's data facility is ~12 EB

Integer Byte Sizes

word size	#bits	range of variable
byte or char	8	256
int	16	65,536
long int	32	4,294,967,296
long long int	64	1.84467440737e+19

Inodes and ZOT Files

- Inodes contain the metadata for files and dirs
- Inodes are pointers to the data
- Regardless of size, a file needs at least one inode to locate it.
- A file of 1 byte takes up the same minimum inode count as a file of 1TB
- DO NOT USE ZOTFILES!! – Zillions of Tiny Files

Editing Big Data

- Use format-specific utilities to view such files and hash values to check if they're identical to what they should be.

- Try not to be the person who tries to open a 200GB compressed data file with nano/vim/joe/emacs, etc.

[De]Compression

- If your applications can deal with compressed data, KEEP IT COMPRESSED.
- If they can't, try to use pipes (|) to decompress in memory and feed the decompressed stream to the app. Many popular apps now allow this.
- Use native utilities to examine the compressed data (zcat/unzip/gunzip, grep, archivemount, Vitables, ncview, etc.

Moving BigData

- 1st: Don't.
- Otherwise, plan where your data will live for the life of the analysis, have it land there, and don't move it across filesystems.
- Don't DUPLICATE DUPLICATE DUPLICATE BigData
- See: <http://goo.gl/2iaHqD>

- rsync for modified data
- bbcp for new transfers of large single files, regardless of network
- tar/netcat for deep/large dir structures over LANs
- tar/gzip/bbcp to copy deep/large dir structures over WANs

Checksums

- They work. Choose one and use it.
- md5sum / jacksum / shasum
- Use MANIFEST files & copy them along with the data files.
- See Checksum example
- http://goo.gl/uvB5Fy

Processing BigData

- Files (HDF5, bam/sam) and specialized utilities (nco/ncview, [Py/Vi]tables, R, Matlab)
- Relational Dbs (SQLite, Postgres, MySQL)
- NoSQLs (MongoDB, CouchDB)
- Binary Dumps (Perl's Data::Dumper, Python's pickle)
- Non-Storage (pipes, named pipes/FIFOs, sockets)
- Keep it RAM-resident.

BigData, not foreverData

- HPC is not backed-up.
- Cannot tolerate old, unused BigData.
- RobinHood is looking for your old BigData.
- Please help us by doing your own data triage.
- Ask your PIs to bug our boss to provide more resources so we can provide more resources.

Remember...

Good Judgment comes from Experience

Experience comes from Bad Judgment

Follow Along

- Take a few moments to login to cluster and follow along if you want.
- After logging in, follow me on screen
- Ref:
- http://moo.nac.uci.edu/~hjm/biolinux/Linux_Tutorial_12.html