UNIVERSITY of CALIFORNIA · IRVINE

Introducing Linux on HPC

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UCI Data Science Initiative

Useful Emails

- Always cc: <hpc-support@uci.edu>
- Joseph Farran <jfarran@uci.edu>
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Course Survey

http://goo.gl/yPS6WK

A General Outline

- Some philosophy.
- Some advice.
- Intro to HPC.
- Intro to Linux
- Intro to the Shell (bash)
- SGE and submitting jobs
- Intro to Biggish Data

I assume...

- You know very little about Linux and even less about cluster computing.
- You can Google & read further by yourself.
- If I speak too fast; let me know
- 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.
- If you code, comment it.

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

- This class will help you do that,

  at least a bit

Getting Help

- Fix IT Yourself with Google <goo.gl/05MnTi>
- Listservs, forums, IRCs are VERY useful for more involved questions
- The HPC HOWTO <goo.gl/kzlql>
- Us – Adam, Harry, Garr, Joseph.
- BUT!! Please ask questions intelligently.

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

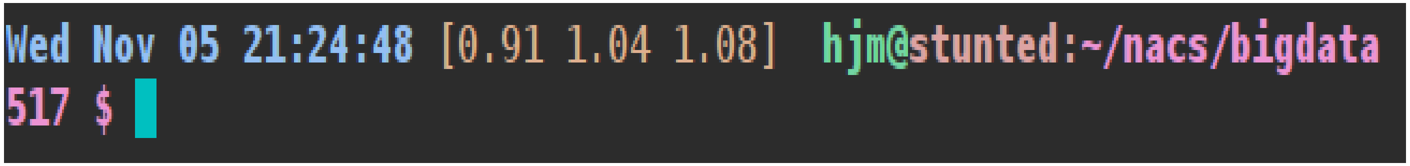
When I submit the job, it appears to go thru the scheduler but then dies immediately when it hits the execution node.

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



```
Wed Nov 05 21:24:48 [0.91 1.04 1.08]  hjm@stunted:~/nacs/bigdata
517 $ 
```

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

On to HPC

What is the High Performance Computing Cluster?

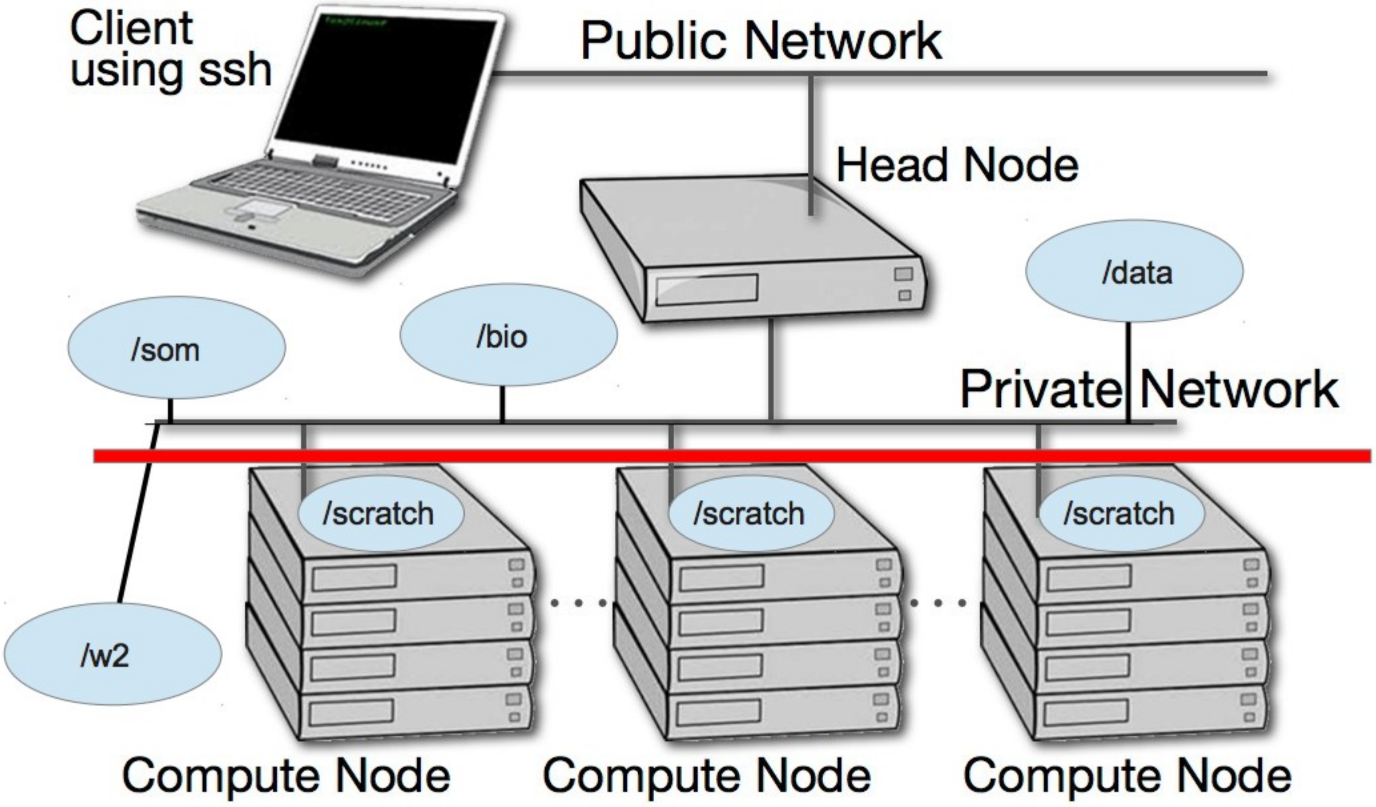
and…

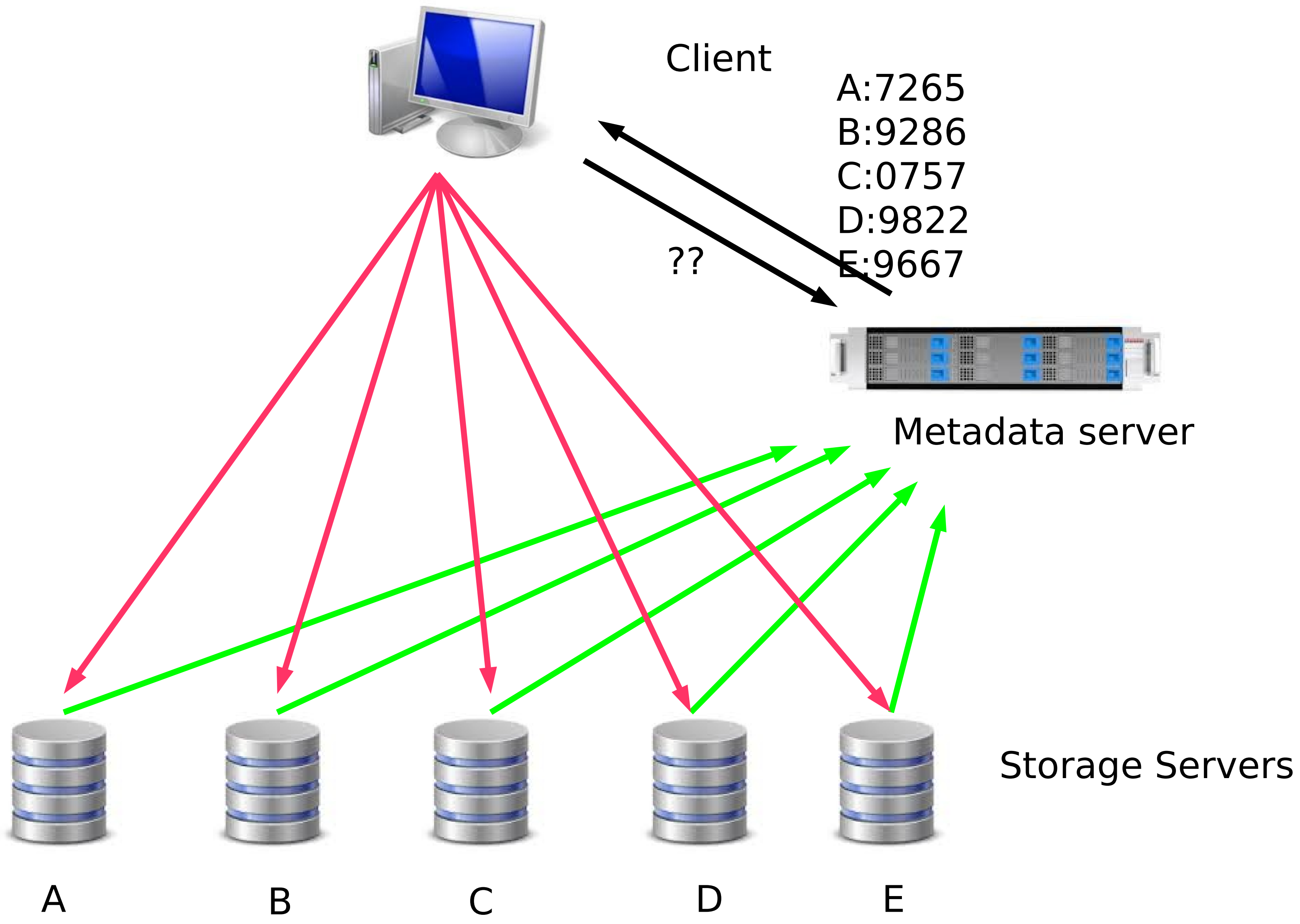
Why do I need HPC?

What is a Cluster?

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

Overview


Client
using ssh
Public Network
Head Node
/data
/som
/bio
Private Network
/scratch
/scratch
/scratch
/w2
Compute Node
Compute Node
Compute Node


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

HPC @ UCI in Detail

- ~5800 64b Cores – Mostly AMD, few Intel
- 4+ Nvidia Tesla GPUs (2880 cores each)
- ~14TB aggregate RAM
- ~1PB of storage (1000x slower then RAM)
- Control network = 1Gb ethernet (100MB/s)
- Data network = QDR IB (5GB/s)
- Grid Engine Scheduler to handle Queues
- > 650 users, 100+ are online at anytime

What HPC is NOT

- NOT your personal machine – shared resource
- NOT BACKED UP – WHAT. SO. EVER.
- Well secured from mischief and disasters – not an invitation

DATA IS NOT BACKED UP

- NO DATA IS BACKED UP – WHAT SO EVER - Agitate to 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
- IF ITS VALUABLE, back it up elsewhere --- or the code that generated it.

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/           More temporary user space
├──── /bio/          Space for BIO group  → /dfs1
├──── /som/          Space for SOM group → /dfs1
├──── /cbcl/         Space for CBCL group → /dfs1
├──── /dfs1/         Fraunhofer FileSystem – new, Distributed File System              ~380TB Space
├──── /scratch       Node-specific temporary storage per job (faster than all above)   ~1TB – 14TB of Space
├──── /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)
- 1yr 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 'differnet' 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

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, or an app that speaks SSH.
- Underlies 'scp' (secure copy), 'sftp'

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!!)

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.

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.
- x2go is described in the Tutorial & HOWTO, also GOOGLE

The bash 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 (csh, tcsh, zsh, perlsh, etc).
- '***bash***' is also a programming language.

Know the shell, Embrace the Shell

- 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 interactive node, with: `qrsh`
- *DO NOT RUN JOBS ON THE LOGIN NODE*

Bash variables

- What's a variable?

- Bash variables are odd.
- Set as THISVAR:

  THISVAR=”jam”
- But read as $THISVAR:

  echo $THISVAR

- Bash is good for *process control* but awful for almost everything else

How to know if I am on Login Node?

- Look at your shell prompt!

```
Mon Apr 28 07:08:59  hmangala@hpc-s:~
678 $
```

- [aebrenne@**hpc-login-1-2** ~]$ ← one of the login nodes
- [aebrenne@**compute-6-1** ~]$ ← On compute 6-1
- May also use the command *`hostname`* to test if you're on a particular host

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
- Use the Tab key for 'auto complete'

STDIN, STDOUT, STDERR

- STD = 'Standard'
- 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, combined, split (by 'tee'), etc
- recombined to make simple workflows
- More on this later.

File & Directories

- Files & folders much like on Mac & Win
- Except...
- Names are case-sensitive, 256 char long, max
- 'Folders' → 'Directories' , separated by '/'
- No spaces in names*
- . means 'in this dir’ (*find . -name thesis**)
- .. means parent dir (*cd ..*)
- ~ means 'home dir' (`ls ~`)
- 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.
- Send a job to the bg by appending **`&`**
- Recall a job to the fg with *`fg`*.
- Send a fg job to the bg with '^z' (suspend), then '*bg*'.
- '*jobs*' - status of your jobs in the current shell

Pipe |

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

Help on Commands

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

Cmds that Inform

- 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 Cmds

- 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 Cmds

- 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

Simple Regex Examples

- 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 session

- Change your prompt to something useful to you (and to us): `PS1="\n\t \u@\h:\w\n\! \$ "`

- Set aliases (`alias nu=”ls -lt |head -22”`)
- Set Environment Variables (`export EDITOR=vim`)
- Use DirB for bookmarks: `source /data/hpc/share/bashDirB`

- Make these permanent via setting them in your `~/.bashrc` file in your *HOME directory*

Editing Text Files

Text editing is not word processing

- Fonts don't count, 'newlines' do, tabs and spaces are different.
- ***GUI-based:***

  gedit, nedit, kate, jedit, emacs
- ***Text-based:***

  nano, joe, vi/vim, emacs

(try them all, 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 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 avail sam`** ditto but starting with 'sam'
- **`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
- **`module whatis`** lists what is known about it

The Scheduler (SGE)

- Just another program that juggles requests for resources
- Make sure your program is working on a small set of test data in 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)

qrsh vs qsub

- *qrsh* will log you into an Interactive Node where you can test out your scripts.
- *qrsh -q queuename* will log you into a node on which you have queue priority.
- These nodes are useful for GUI programs (X11 or 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 with NO USER INVOLVEMENT during the process.

SGE – Queues

- The scheduler uses different *queues* to handle your job.
- Some queues have higher priority than others, depending on who you are.
- Type '`queue`' or '`q`' to see what you have access to.
- `#$ -q som, free*`

SGE 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

- You MUST read this before starting to submit jobs:
- http://hpc.oit.uci.edu/running-jobs

SGE – Request Node Resources

- You're in SoM & know your program requires
- 24GB Memory
- 16 CPU Cores
- You need to include in your qsub script:

  #$ -q som,asom

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

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

SGE – Free and All Queue

- The free* queues 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 or migrated off.
- Please see: <http://hpc.oit.uci.edu/queues>
- Similar to the free* queues, the 'all' queue is group-specific: abio, asom, etc.

SGE – Checkpointing

The Berkeley Checkpointing system allows jobs to:

- Be bounced to another node when it gets suspended
- Survive crashes since it checkpoints the job state every 6hrs, so it will never lose more than 6 hrs of runtime.
- Avoid the runtime limit by resubmitting the job back into the job queue.
- BUT, your qsub script needs to request the setup beforehand – only 2 directives required.

- See: <http://hpc.oit.uci.edu/checkpoint>.

GE – Job Arrays

Job Arrays allow a single job to act as if it is operating in a loop.

- You can use the built-in counter **$SGE_TASK_ID** to control the sequence of jobs
- You can control the job by referring to only 1 JobID.
- It is MUCH more efficient to do 1000 jobs via Job Array than by individual qsub.
- An efficient alternative to script generators.
- So if you have zillions of almost identical jobs and can index them via the **$SGE_TASK_ID** counter, then use Job Arrays

QSUB Scripts

- Some useful SGE script parameters <http://goo.gl/hrcXBg>
- Example qsub scripts:

  <http://goo.gl/ENsBYt>

Big Data

- Volume

  Scary sizes, and getting bigger

- Velocity

  Special approaches to speed up analysis

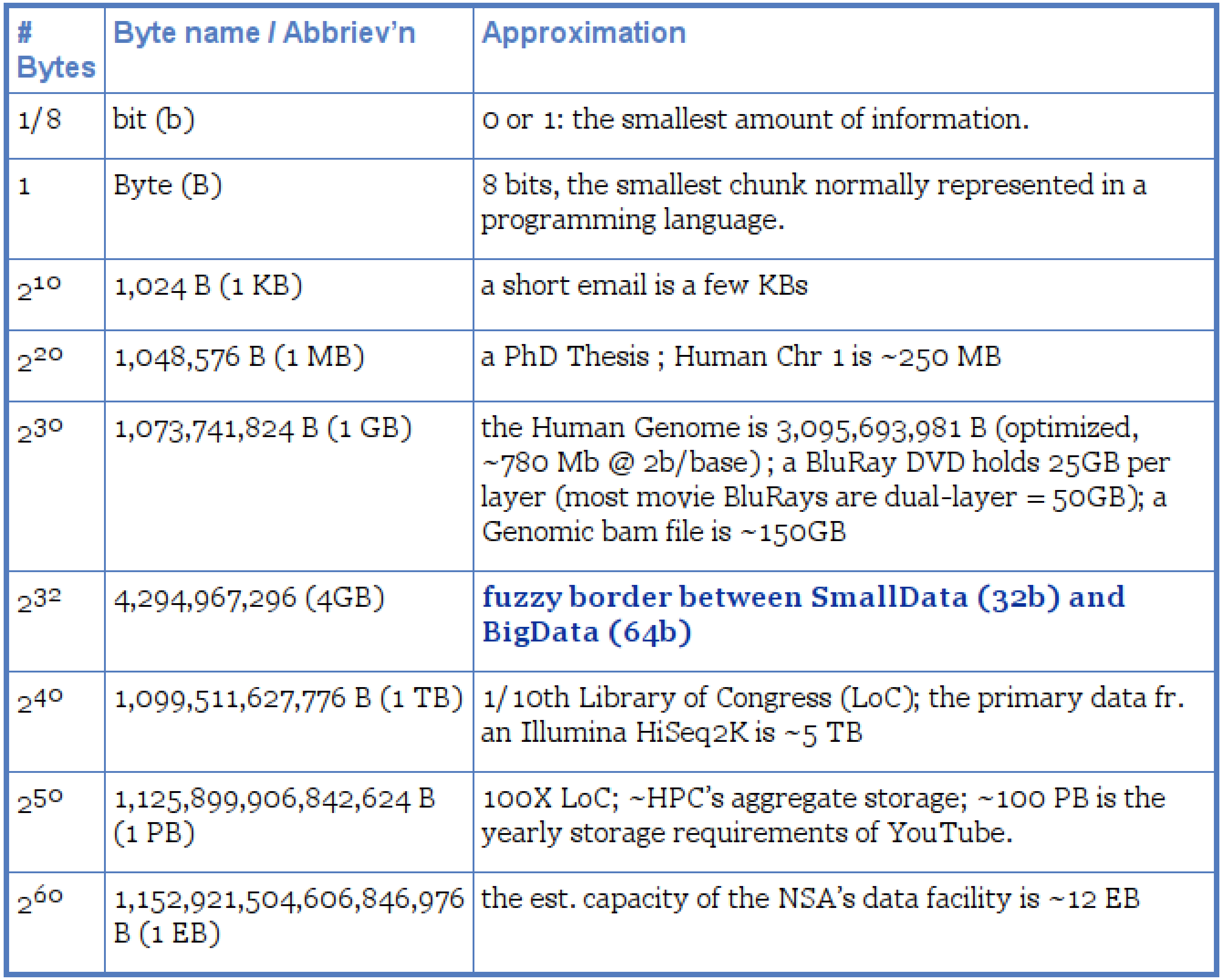
- Variety

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

- BigData Hints for Newbies

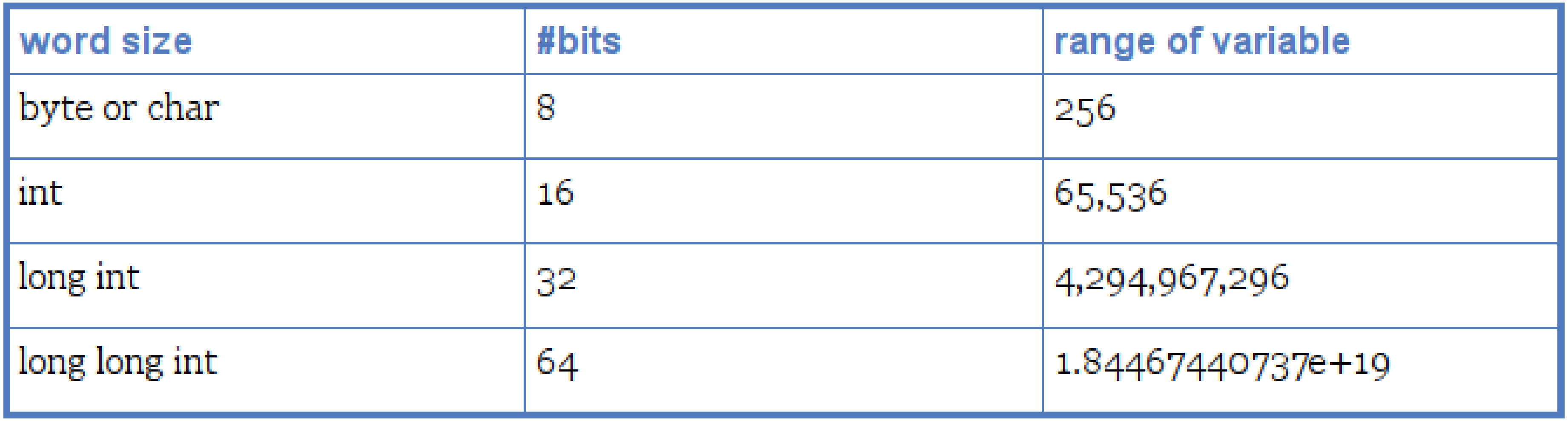
  <http://goo.gl/aPj4az>

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

Streaming Reads & Writes

Let me demonstrate with a card trick.

Pointless Data Replication

- How informative is this?
- How informative is this?
- How informative is this?
- How informative is this?
- How informative is this?

vs

- How informative is this? [5x]

Editing Big Data

- Don't

- 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
- Automatically generate 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.

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