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Faculty of Arts and Sciences
RESEARCH COMPUTING

Introduction to Odyssey

Bob Freeman, PhD
RC Facilitator
XSEDE Campus Champion

robert_freeman@harvard.edu
@DevBioInfoGuy

Goals

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Objectives

- Help you to understand the complexities of our services and frame our role in the services landscape
- Use compute resources efficiently
- Submit jobs without affecting the work of 500+ other active users
- Reduce the support burden on the RC/Informatics team

Strategically

- “Work smarter, better, faster”
- ... and to Think Differently
- Demonstrate leadership in advanced technologies
- Foster collaborations across institutional boundaries
- Enable you to be successful with your research!

Overview

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1. RC & Informatics People
2. RC & Informatics Services
3. Beyond RC: XSEDE
4. Consulting/Training
5. ACI & All About Odyssey
6. Typical Workflow
   a. Login & Access
   b. Filesystems & Storage
   c. Transferring Files
   d. Loading Software
   e. Login/Interactive Nodes
   f. Choosing Appropriate Resources
   g. Submitting/Controlling Jobs
7. Troubleshooting
8. Common Pitfalls
9. Getting Help

Slide deck avail as PDF after class

People of RC & Informatics

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- 20 people (leadership, cloud, sysadmin, client support)
- Strong overlap with Informatics group (10 in leadership, web, science, sci/code)
- Ph.D.s in biology and physics, w/ roles as sysadmins and developers
- Supporting ALL sciences & major HU computing projects (BICEP2, ATLAS, etc.)
- Also support SEAS, HSPH, & HBS

RC Services

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Odyssey (cluster)	~60K compute cores (CPUs) and increasing *high-throughput / high-performance computing*
Storage	14 PB private, shared, and scratch storage; and increasing *Lab and personal data; scratch/work temporary space*
Visualization	65+ GPGPUs and increasing *high-end visualization; real-time interactive rendering*
Virtual Machines	~600+ KVM images *Web portals, license or server-based resources; restricted datasets*
Apps/Libraries	>3000, in chemistry, biology, statistics, social sciences, & others *Predominantly cluster-based & open source; some desktop/licensed*
Other	Database hosting Application licensing Workflow & Code optimization Instrumentation & Core facilities support Consulting
HUIT	Networking, student computing, admin apps, & desktop support

All services are free except private compute and private (lab) storage

Informatics Services

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Core facilities-associated activities:

- Primary sequence analysis i.e. basecalling/multiplexing
- Sequence data QC/trimming
- Alignment to reference genome
- Bioinformatics software installation/support
- Consultation and recommendations for amount and type of sequencing
- Consultation and recommendations for sequence analysis

Non-core activities:

- Transcriptome assembly and differential expression analysis
- Whole genome assembly and genome comparison
- Annotation of assembled transcriptomes
- Database construction
- SNP calling and filtering
- Custom script/algorithm writing
- Phylogenetic analysis

We are happy to meet and help people get up and running with these things.

RC & Informatics Training

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Training opportunities: New & Evolving…

- Office Hours: every Wed 12 - 3 pm @ RC conference room
- Tips@12: Highlighted topics in the first ½ hour of Office Hours
  - Troubleshooting Jobs, iPython Notebooks, Parameter Sweeps, Unix Tricks
- *Intro to Odyssey & RC Services*
- Next Steps… / Parallel HPC series (early 2016)
- Guest lectures in courses
- Lab-specific, customized training, including optimizing workflows
- MATLAB workshops (Fall '14, Spring '15)
- Software Carpentry (http://software-carpentry.org/ Fall '14, Summer '15)
- Data Carpentry (http://datacarpentry.org/ Summer '15)

All of the training materials can be found at http://fasrc.us/fasrcmaterials

Consulting & Outreach

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- Consulting

  Given appropriate expertise, some significant engagements to help with code and analysis optimizations are possible

- Adv CyberInfrastructure – Research & Education Facilitation

  Special 2-yr NSF grant for cluster computing education/facilitation

  Partner with you to enable your research: use compute resources, work more efficiently, and be more competitive

  Collaborations: Clemson U., U. Southern California, U. Utah, U. Wisconsin (Madison), U. Hawaii

  HU FASRC: Bob Freeman, PhD

http://aciref.org/

ACI-REF Advanced CyberInfrastructure Research & Education Facilitators

NSF

Example Workflow Improvements

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- Transition to HPC from GUI
  - video processing workflow, all GUI driven
  - uses ImageJ and MATLAB, with 6 streams and ~10 steps
  - in progress, but down to 30 minutes from 12 hrs
- Video processing workflow
  - complex cluster pipeline for tracking animal movements
  - custom code developed by post-doc who left; no version control
  - in progress, adapting to current cluster, version control, & multicore processing
- Recoding of geophysical simulations
  - visco-elastic models for simulating earthquake movements
  - transitioned from MATLAB to fortran, & parallelized code via MPI
  - reduced compute time to 10 hrs from weeks

ACI-REF Advanced CyberInfrastructure Research & Education Facilitators

NSF

Beyond RC: XSEDE

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- Umbrella organization for 16 supercomputers and high-end visualization and data analysis resources across the country
- 5-year, $120m project funded by NSF & successor to TeraGrid
- Campus champions exist to help you apply for and take advantage of these off-campus resources (HU: Bob Freeman)
- Can use XSEDE & RC resources simultaneously
- https://www.xsede.org/
- Excellent training resources for *everything HPC* with portal account (open to everyone)
- Eligibility: NSF-funded grad students, post-docs, and faculty
- Education, Startup, and Research accounts

From **Profiles in Delight: Paul Edmon** (ITC RC Assoc):

What's the biggest misconception about RC or HPC in general?

That if you just put your code on the supercomputer it will run faster. As it turns out the processors we use on the cluster are not much better than what you have in your desktop. At times your desktop may be faster. What makes HPC work is that we have a vast number of these processors all networked together with a high speed interconnect. Not even sending it to the cloud will get you that.

In order to get the most out of your code and leverage any HPC resource (whether it be ours, the cloud, or XSEDE) you need to optimize your code and workflow. This takes time and effort. You need to learn about the hardware you are running on, the code you are running, the science you need to get done, and marry all that together to make sure you get things done as quickly and accurately as possible. Supercomputing isn't a blackbox, and the more you understand the better you can engineer your workflow and code to take advantage of the great resources we have available. We at RC are here to help people achieve that.

Advanced Computing Capabilities

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At Harvard, to facilitate your computing capabilities, RC provides

- Physical infrastructure: power, cooling, and space
- Expertise for system administration, algorithm/programming support, & technical advice
- Economies of scale

Value to you??

- Groups can purchase dedicated hardware or use the general resources
- Leads to better and more efficient use of resources:
  - Easier entry into the world of HPC
  - Groups who own resources get priority on the resources they own
  - Others get to make use of the spare cycles when the resources are not in use

Who can benefit from HPC?

- If your analysis takes longer than 10 min on your desktop/laptop
- If you're doing tens/hundreds of tasks
- Analyses using a GUI that could be done at the command line
- Datasets requiring large RAM or large numbers of compute cores

As HU pays for infrastructure costs whether machines are busy or idle, fully utilized machines are a very good thing!

What is Odyssey?

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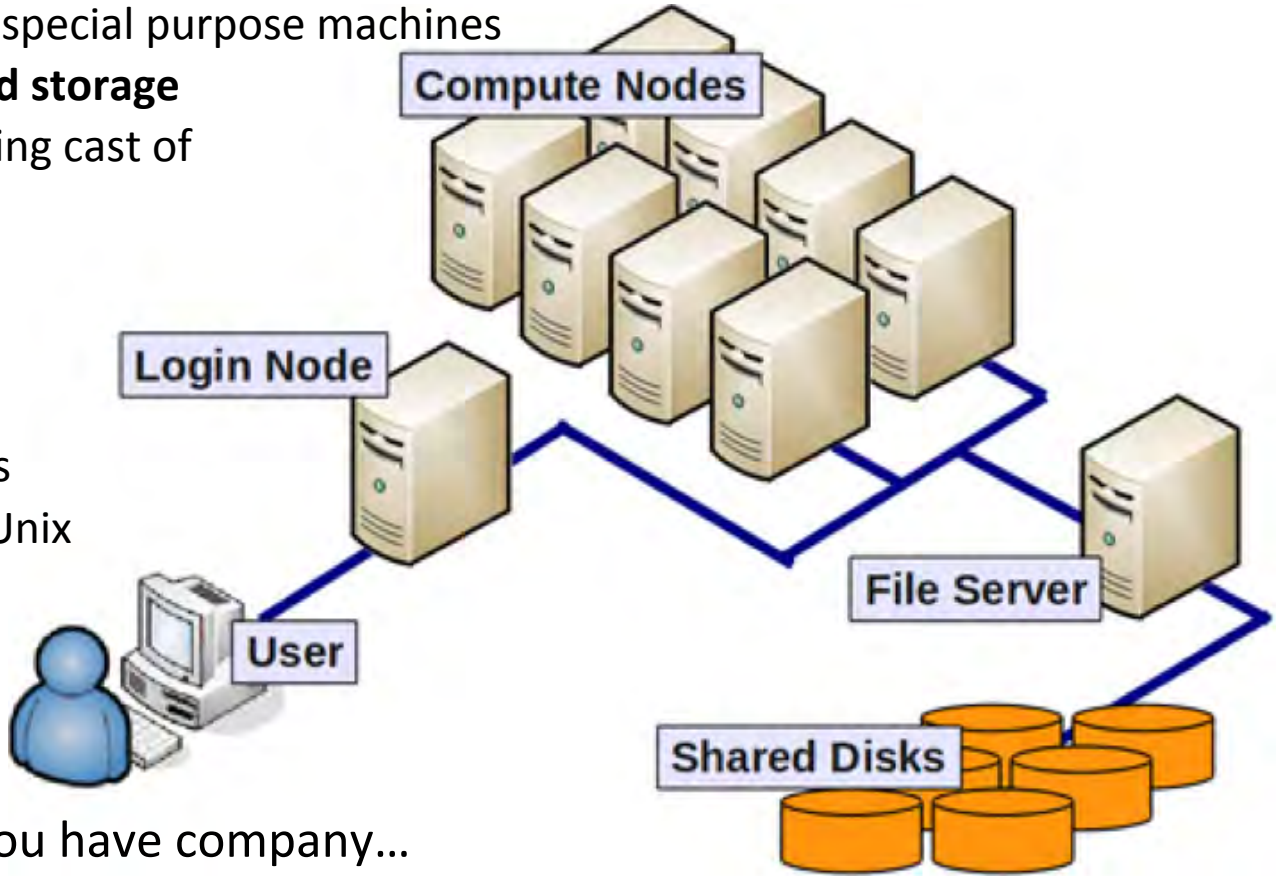
RC's premier resource is the Odyssey cluster. What is a cluster?

A collection of various types of hardware:

- A cluster of tightly interconnected **machines with identical hardware**
- Several high-powered, special purpose machines
- Large amount of **shared storage**
- Miscellaneous supporting cast of other servers

And some software:

- **User and group management:** separation of resources
- **SLURM** (Simple Linux/Unix Resource Manager)
- Linux OS (CentOS 6)

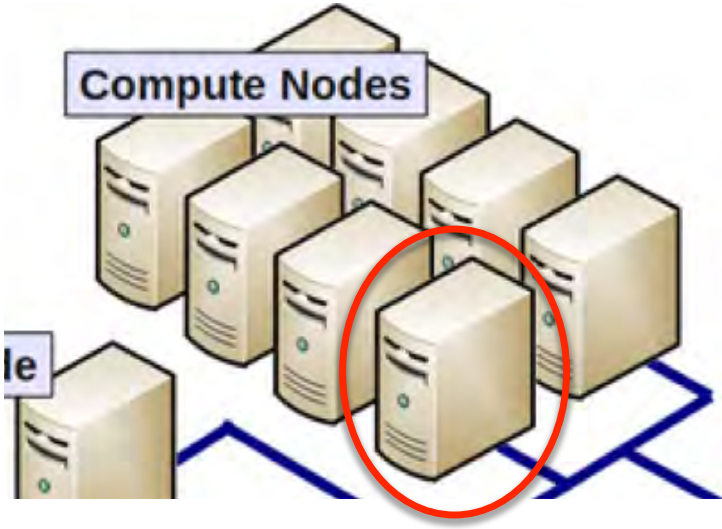


It's a **shared** system -- you have company…

Key definitions...

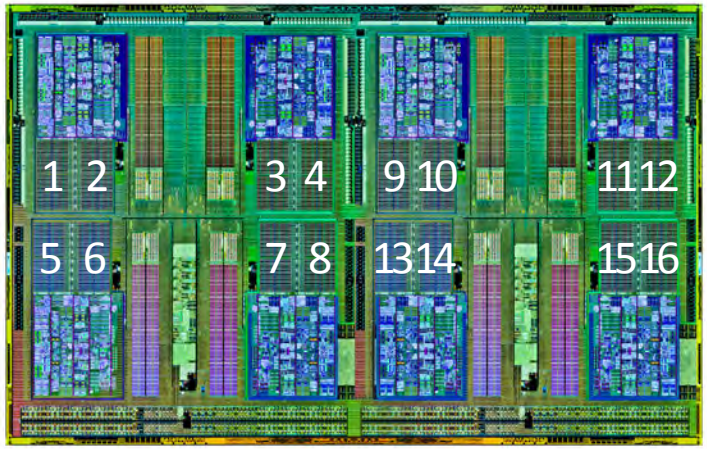
The typical hardware unit is called a **node**

- Same stuff that's in a desktop/laptop: CPUs, Memory, Hard drive, Network cards
- But more powerful and more of them compared to a typical desktop
- Nodes are individual hosts with distinct names. E.g...
  - rclogin03: one of the login nodes, located either in Boston (60 Oxford St or 1 Summer Street)
  - holy2a18208: one of the compute nodes, located in Holyoke, MA



The basic computational unit in a cluster is a **CPU core**

- Each core runs one process, a *average* job
- Most compute nodes have 64 cores arranged on 4 CPUs (16 cores/CPU)
- Thus, most nodes run 64 batch job processes



Key definitions...

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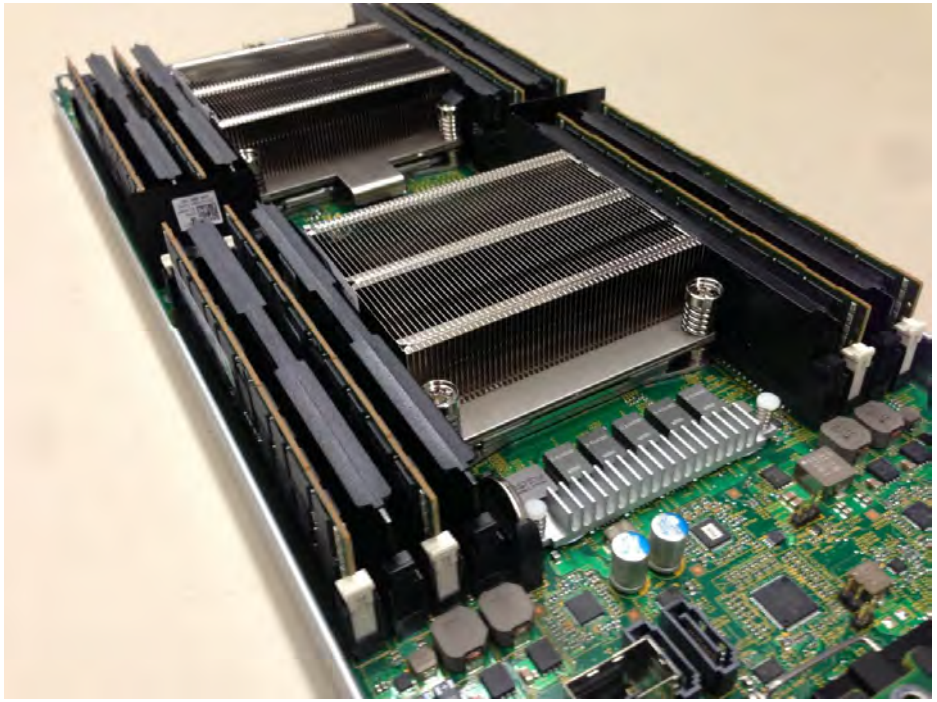
A **typical compute node** is configured:

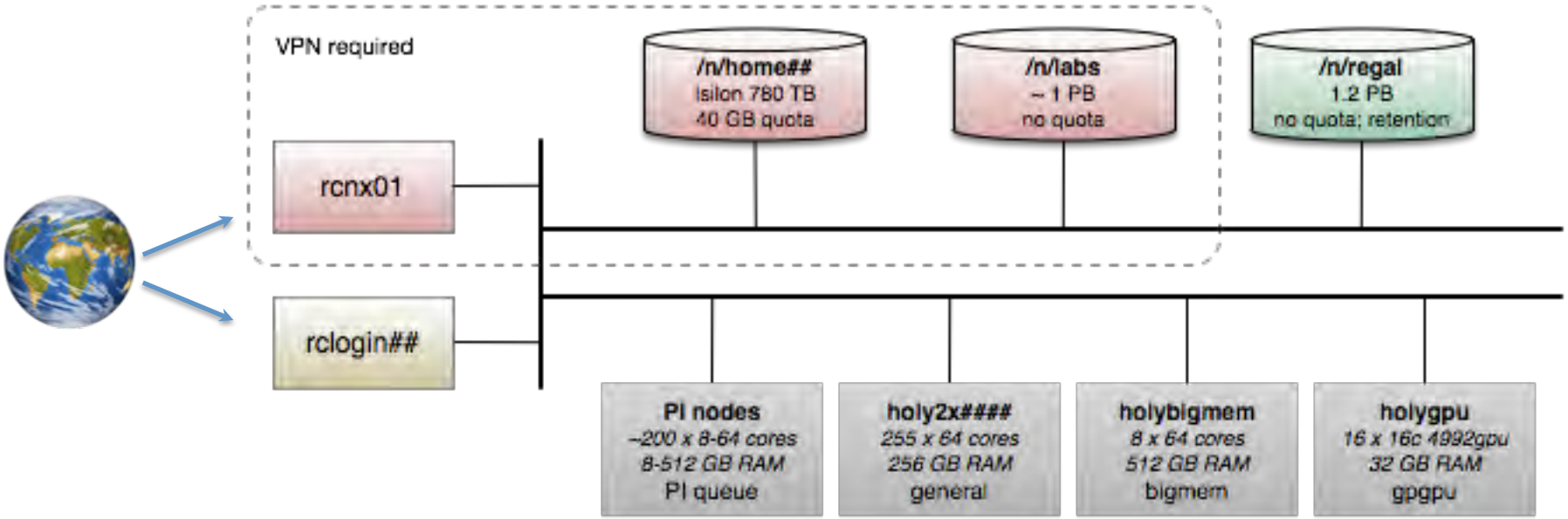
- 64 cores
- 256 GB RAM, or ~4 GB RAM/core
- 2 network cards:
  Infiniband (intraconnect)
  & xGb connections (interconnect)
- Small, local hard disk/SSD
  for boot and local /scratch



All cores on a node share all other resources of the node: memory, network bandwidth, etc.

Thus, how you use these resources affects the other 63 jobs on that compute node

What is Odyssey?



https://rc.fas.harvard.edu/odyssey/

What is Odyssey?

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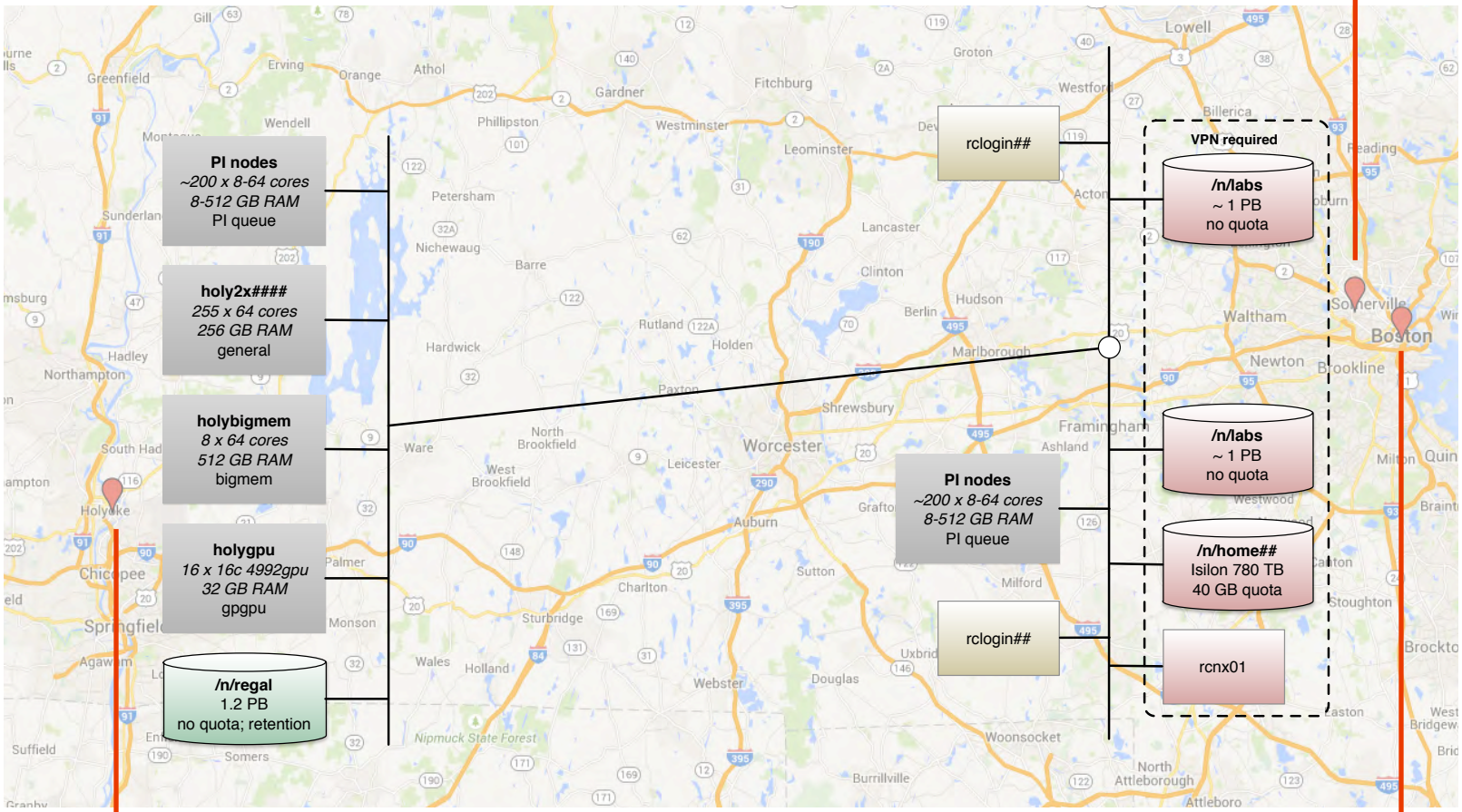
Compute nodes/disk are located in 3 data centers:

60 Oxford Street



MGHPCC, Holyoke MA

1 Summer Street

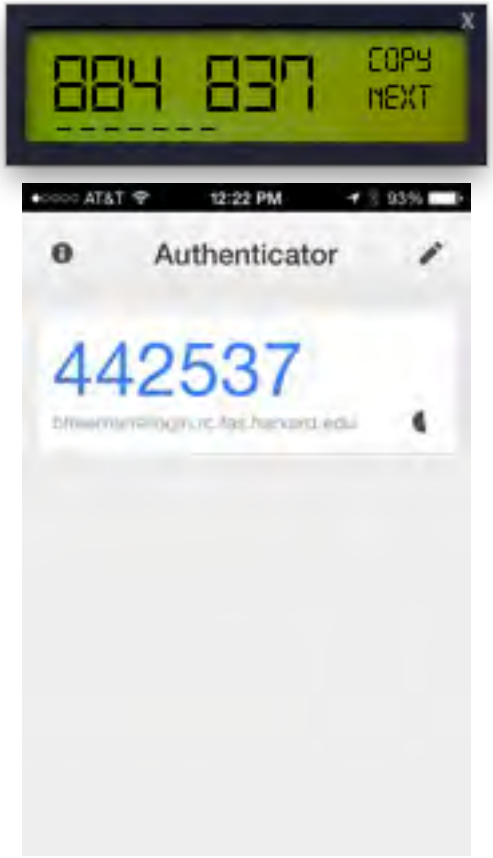
Topology may effect the efficiency of work

Typical Workflow

1. Login in to Odyssey
    a. Land on a login (head) node, appropriate for light work only
2. Copy/upload/download some files
3. Load appropriate software
4. Get interactive session
5. Test your program/script interactively to ensure it runs properly
6. Test run in batch: create batch file & submit to SLURM
    a. Continue working in the foreground while waiting for results
7. Scale up as necessary (10s, 100s, 1000s)
    a. With *caveats*: proper file placement, # cores, etc.

Login & Access

- Use your RC credentials for:
  - Instrument Windows machines
  - VPN
  - File transfer clients
  - Mounting disk shares
  - Terminal sessions to Odyssey
- OpenAuth 2-factor authentication (2FA) required for VPN & Odyssey sessions (file transfer & terminal)
- Account locks automatically if 5 failed login attempts, and auto unlocks after 10 minutes
- **Reset your own password** on RC portal
- If you are switching labs, please let us know, as we'll need to change your access groups



Account credentials should not be shared!
Using RC services in an explicit acceptance of the University Security Policy
http://security.harvard.edu/book/information-security-policy

Data Security: Storage/Use of HRCI

Confidential data is defined as

> "Information about a person or an entity that, if disclosed, could reasonably be expected to place the person or the entity at risk of criminal or civil liability, or to be damaging to financial standing, employability, reputation or other interests."

See HU's IT Security pages for methods for handling & network access: http://security.harvard.edu/

Under no circumstances should HRCI data be stored on RC storage without consultation. Storage must be specifically designed for HRCI data: http://fasrc.us/data_hrci

Working on restricted datasets (e.g. dbGAP or CMS)?

- Set up a follow-up appointment with RC
- Requires discussion and training on facilities you/PI can access under the University Data Usage Agreement (DUA) process
  - DUAs: Important documents signed by PI and Asst. Dean of RC to protect important datasets
  - Each dataset / DUA must be handled in a unique manner
- http://vpr.harvard.edu/pages/harvard-research-data-security-policy

Your PI must brief you on training for these datasets and how they need to be controlled

Login & Access

Recommended SSH clients:

- Terminal on Mac/Linux
- Putty on PC
- XQuartz (Mac) or Xming (PC) for X11

```
ssh rcusername@login.rc.fas.harvard.edu*

# Or, if X11 forwarding is required...
ssh -YC username@login.rc.fas.harvard.edu
```

We expect you to have good Unix skills before submitting jobs on the cluster. See http://fasrc.us/unixfoo

*unless in sensitive information setups

Getting Good Unix Skills

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We expect you to have the following Unix skills before submitting jobs:

- Know how to traverse directories
- Know how to create & remove files & directories
- Know how to copy/move files & directories
- Know how to edit a file using a simple text editor like nano, vi, or emacs
- Read and write files with commands like head, tail, cat, and less
- Understand and modify unix file/directory permissions
- Understand I/O redirection
- Have some basic understanding of $PATH and what login files are for

If you cannot perform all these functions, please review any of the following materials:

- RC's John Brunelle's ComputeFest2014 Unix Intro

https://software.rc.fas.harvard.edu/training/workshop_intro_unix

- Unix screencast from our ACI-REF collaborators at UClemson

http://citi.clemson.edu/training/ (links in center of page)

- HUID account holders have access to all of Lynda.com's training:

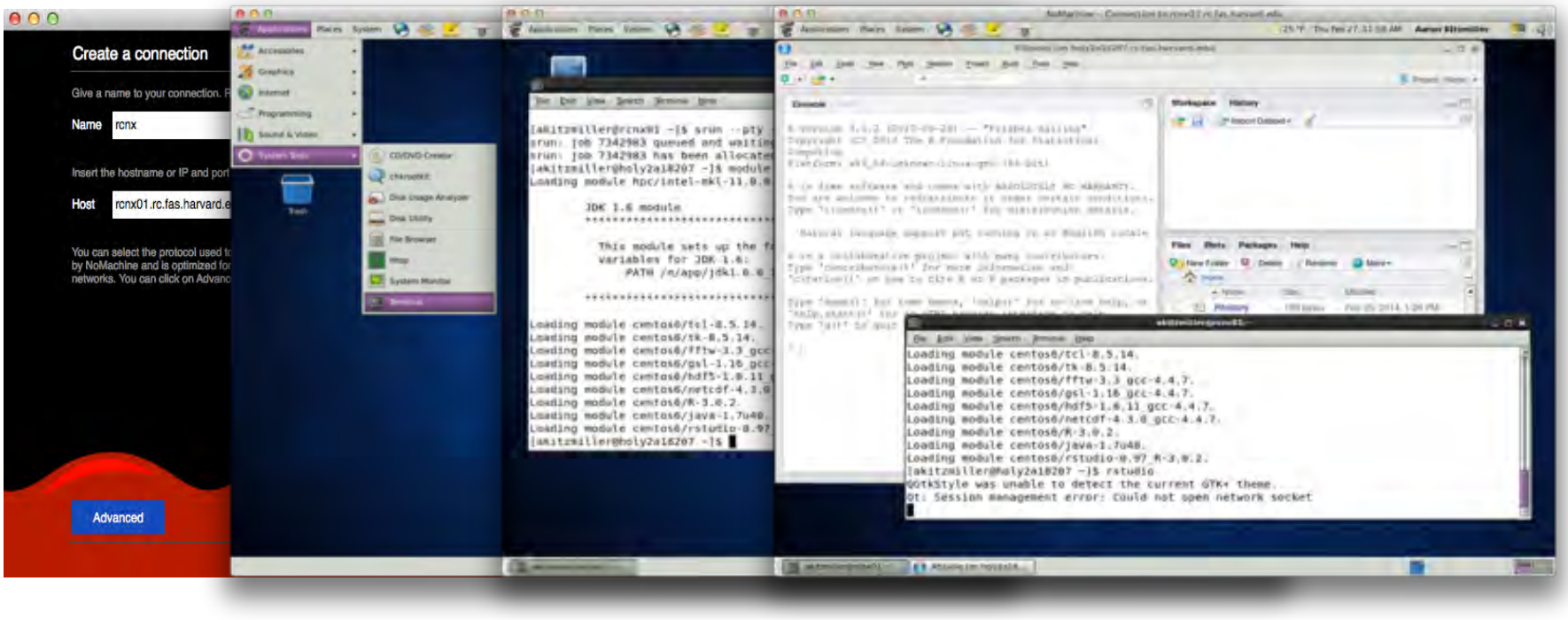
http://ohrdb.harvard.edu/cwdcourses/description.php?recordID=324

- Software Carpentry's 'helping lab people compute smartly' Unix Intro:

http://software-carpentry.org/lessons.html

GUI Login

- Some apps require GUI/X11 interface: MATLAB, RStudio, CLCBio, etc..
- Use NoMachineX instead, as X11 performance can sluggish
- *VPN is required* (vpn.rc with username@odyssey* + 2FA)
- As rcnx01 and holynx01 login nodes, *request an interactive* session after login to do any work



* exception is for sensitive information setups

Transferring files to/from Odyssey

GUI client Filezilla for all platforms

- Configure according to http://fasrc.us/configfilezilla to avoid 2FA problems

Command line tools `scp` or `rsync`

- `rsync` is best for resuming transfers or transferring only changed file parts

Download data using `curl` or `wget`

- is available on all compute nodes, though web proxy needed for HRCI setups

Or by mountings disk shares. Please see http://fasrc.us/mountdisks

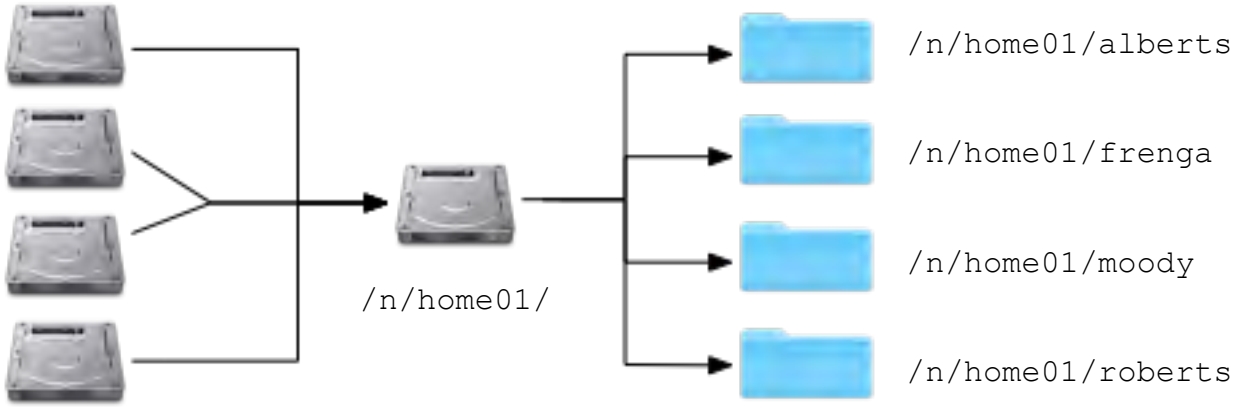
Examples:

```
# copy file in current dir to Odyssey home folder
scp somefile.txt rcuser@login.rc.fas.harvard.edu:~

# copy folder in current dir & contents to Odyssey home folder
rsync -av myfolder rcuser@login.rc.fas.harvard.edu:~

# download FASTA sequence from NCBI
wget "http://www.ncbi.nlm.nih.gov/nuccore/L03535.1?report=fasta&log$=seqview&format=text"
```

Filesystems & Data Storage



Storage on Odyssey is not what and where you think it is…

- Created by bundling together a group of disks to form a virtual volume
- The virtual volume is sliced up into one or more filesystems to hold files & folders
- These are accessed transparently over the network through *mount points* (e.g. `/n`)

Running large #s of jobs out of home or lab directories will negatively affect all other persons sharing those physical disks

Take home message: Ensure that you use the proper filesystem for your work

Common Filesystems

	Type	Size	Avail?	Mount Desktops?	Backup?[1]	Retention?	I/O profile
`/n/home##`	NFS	40 GB (hard limit)	all nodes	Y	Y	N	low
`/n/labfs#`	NFS	1 TB free (new labs) contact for costs	all nodes	Y	Y [2]	N	low
`/scratch`	local	250 GB/node (~4 GB/core)	all nodes	N	N	Y[3]	high
`/n/regal`	Lustre	1.2 PB	all nodes	N[4]	N	90-days[5]	high

[1]Backup methods differ. See http://fasrc.us/faqrecovery for more information.
[2]Lab disks shares are typically backed up unless noted.
[3]Files usually deleted when job finished. Please clean up your own mess, though.
[4]Can use file transfer methods to stage data.
[5]Retention is typically run at maintenance times. Areas can be exempted for common data (e.g. NCBI Genbank at `/n/regal/informatics_public`). Contacts us.

Common Filesystems: /scratch

Using local `/scratch`:

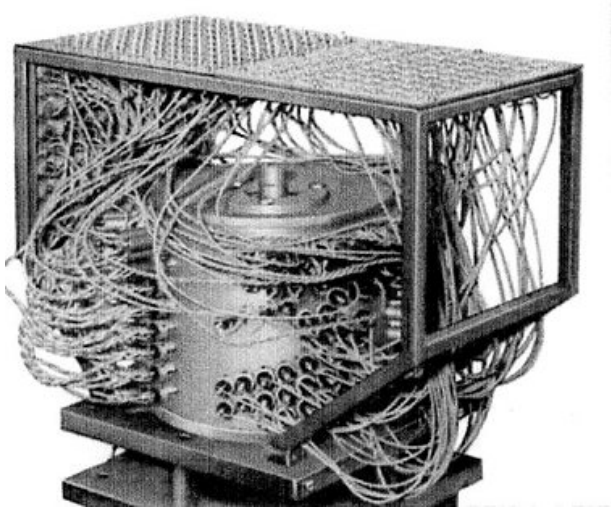
- 250 GB slice on each compute node, so there's about 4 GB disk space/job
- Is currently underutilized, so more space may be available (check `sbatch` options)
- Can see speedup of 2x – 3x, depending on pattern of file read/writes
- Since is local to each node, must use it *during* your job:

```
...
start_dir=$PWD
mkdir -p /scratch/$USER/$SLURM_JOBID
cd /scratch/$USER/$SLURM_JOBID

# do your work while writing temp files here
...

# copy files back and return from whence we came
cp –r results/ $start_dir/
cd $start_dir

# now cleanup
rm -rf /scratch/$USER/$SLURM_JOBID
```



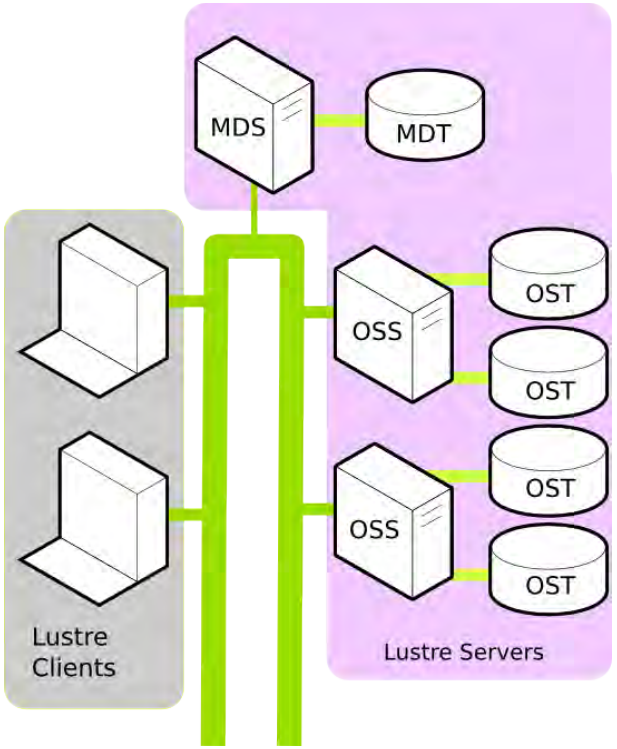
Common Filesystems: /n/regal

Using `/n/regal`:

- Most work should be done here, especially for ~≥ 10 simultaneous jobs
- No space restrictions, but files > 90 days old deleted (usually at maintenance)
- Can stage files prior to job by typical copy/rsync commands or Filezilla
- Remember to copy results back to home or lab shares for permanent storage

A couple more things to remember:

- Shared lab areas can be exempt from retention. Contact us.
- Public data sets can also be staged here – no need to keep your own copy
- NCBI, EMBL, UCSC data is stored at `/n/regal/informatics_public`:
  - FASTA data, BLAST databases, Bowtie2 indexes
- Contact us if you'd like to add more to this location



Load/Installing software

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We have ~3000 applications/libraries in chemistry, biology, statistics, social sciences, and more available for use, but not at all the same time

Software is loaded incrementally using modules, to set up your shell environment

Rolling out a new module system `Lmod`:

- New system is opt-in for old accounts, but will be default soon (if not already)
- Strongly suggested reading: http://fasrc.us/rclmod

```
source new-modules.sh                    # for opt-in folks
module load fastqc/1.0.0-fasrc01         # specific version

module load fastqc                       # most recent version

module-query fastqc                      # also --full-text option
module spider fastqc                     # find details on software
module avail 2>&1 | grep -i fastqc       # find software titles
```

Software search capabilities are also available on the RC Portal!

Load/Installing software

Old (legacy) modules system still available, but use is **highly** discouraged…

```
module load legacy                      # get to old modules
module load centos6/bowtie-1.2.1        # old can be used with new
```

If not using `Lmod` , the old (legacy) module system still available, but will be retired soon

These modules are at http://fasrc.us/modulelist, or

```
module avail 2>&1 | grep -i 'fastqc'    # find software

module load centos6/fastqc-0.10.0
```

Module loads best placed in SLURM batch scripts:

- Keeps your interactive working environment simple
- Is a record of your research workflow (reproducible research!)
- Keep `.bashrc` module loads sparse, lest you run into software and library conflicts
- Use small source or script files to do complex module loads

Load/Installing software

Please only request software installs if the program will be used by multiple labs or if standard in your domain.

For all other software, please install software yourself

- Follow software instructions for 'local', non-root, or 'home' directory installation
- Consult our web site for instructions on using appropriate compilers
- Please don't use the `sudo` command

For Perl / Python modules or R packages

- Installation can be in home folder (personal) or lab folder (shared)

Consider using home folder for personal or for code under development; and lab folder for code in shared projects or production code

NB! Do not request software installs for Java apps and Python scripts. These should be installed yourself per developer's instructions

Details at http://fasrc.us/installsw

Login vs Interactive Nodes

Terminal sessions to `login.rc` puts you on one of several login nodes

- This gateway to the cluster has limited entry points, so..
- Only non-CPU-intensive work is appropriate: `cp`, `mv`, `nano`, `rsync`, etc.
- *Reminder*: rcnx01 and holynx01 are login nodes

Don't compute here, instead

- Submit a batch job (background task) to SLURM, or
- Request an interactive session (foreground task) on a compute node:

```
srun --pty --x11=first --mem 1000 -p interact -t 0-6:00 -n 1 -N 1 /bin/bash
```

srun: foreground
sbatch: background

Resources that you wish to request from SLURM

Script or program
`/bin/bash` == shell

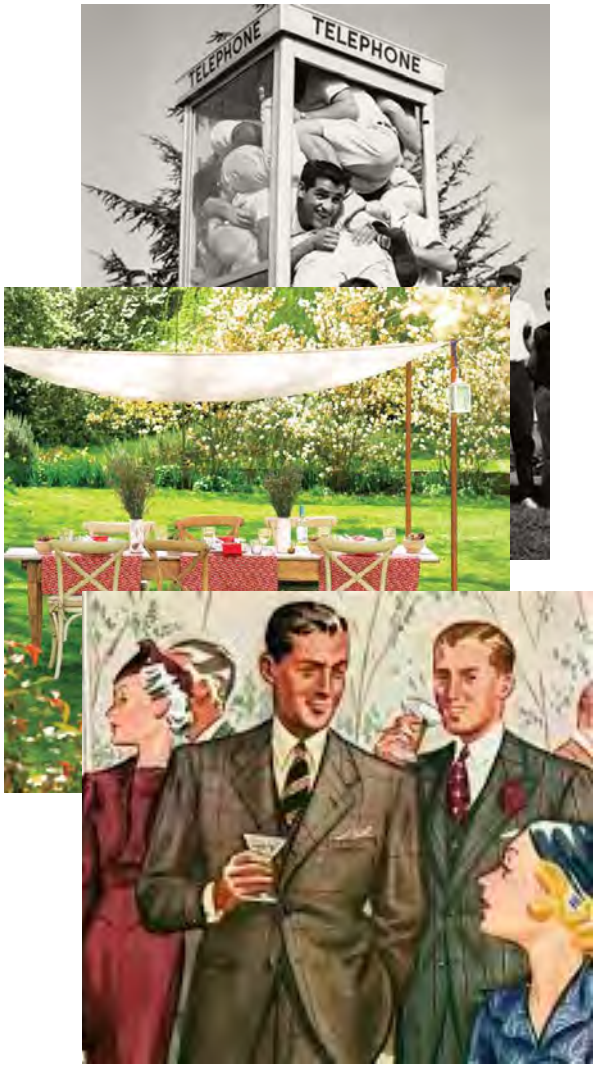
Choosing Resources: How?

Choosing resources is like attending a party:

- You need to RSVP the number of guests you intend to bring
  Request the resources you intend to use
- Extra guests: there's not enough food and drink for everyone
  CPU/disk overage: all jobs including your will run more slowly
  RAM/time overage: your job will be killed
- Too few: an unhappy host and wasted $$ / effort
  CPU/RAM: resources are wasted as they cannot be used by anyone else
  All: your job becomes harder to schedule

You also want to be polite:

- Stay the appropriate amount of time…
  Try to approximate your resource use with some padding for safety
- Don't slip in, drink & eat, and leave within minutes
  Try to avoid jobs that start and complete within minutes; especially in large numbers



Choosing Resources: Time & Memory

Time:

- Determined by your test runs during an interactive session
- Or if trying in batch, over-ask first, then reduce time on later runs
- Due to scheduler overhead, jobs should do at least 5 - 10 min of work

Memory:

- Check software docs for memory requirements
- If none stated, over-ask and do a trial run (via `srun` or `sbatch`)
- use `sacct` command to get post-run job info:

```
# RAM                                    requested/used!!
sacct -j JOBID --format=JobID,Elapsed,ReqMem,MaxRSS
```

"Never use a piece of bioinformatics software for the first time without looking to see what command-line options are available and what default parameters are being used"

-- acgt.me · by Keith Bradnam

Choosing Resources: Partitions

Name	Length	Size (cores)	Memory/node	Usage
interact	3 days	512 (8 nodes)	256 GB	all interactive work
serial_requeue	7 days*	30K+	varies (512 GB max)	best for single core jobs; or small numbers of cores for short durations; schedules best as hits all parts of the cluster
general	7 days	~14K	256 GB	large # of cores; MPI jobs; jobs sensitive to pre-emption (pipelines)
unrestricted	no limit	512	256 GB	all jobs with no time limit
bigmem	7 days	512	512 GB	jobs requiring >256 GB RAM (restricted access)
(private)	no limit	varies	256 GB typical	lab-specific partitions

Note: SLURM can schedule to quickest of two partitions with `-p partion1,partion2`

Choosing Resources: Partitions

interact

- Use for foreground, interactive sessions up to 2 days
- You can request multiple cores or large RAM
- Limit the number of active, interactive session to 5 or less

(private)

- PI-specific partitions, usually named after the lab
- Access is automatic, by group membership

bigmem

- For work where each job requires > 256 GB RAM
- Accessible only by request

general

- For all large core #, long, or MPI jobs, or jobs sensitive to pre-emption
- When busy, typically will take tens of minutes or hours to schedule
- Requesting full nodes may take >1 day for your job to schedule

Choosing Resources: Partitions

serial_requeue

- Recommended partition for single-core jobs; or jobs using up to 8 cores lasting up to approx. 6 – 12 hrs
- Most 'powerful' as hits every core on the cluster, including private compute
- Dispatches within seconds to minutes

But the downside…

- Jobs may be pre-empted (killed) if originally scheduled on a private node and the node owner submits work. **Your job is automatically rescheduled**

To mitigate this…

- Use the sbatch option `--open-mode=append` for your `-e` and `-o` log files
- Use `%N` (in addition to `%j`) in log file names to indicate what host your job ran on.
- If you append output, ensure that you zero your data files at the start of the job, to ensure that any files left over from a previous, partial run are removed.
- Structure your command flow so that you skip over any work already done. This allows your re-run job to pick up from where the pre-empted one left off.

Submitting jobs

Two methods for submitting jobs via `sbatch`…

For simple, one line commands, submit with `sbatch`:

```
sbatch -p serial_requeue -n 1 -N 1 -t 0-1:00 \
--mem 100 -o hostname.out -e hostname.err \
--mail-type=ALL --mail-user=rmf@123.com \
--wrap="rsync -av ~/test/some_set_of_files \
        /n/regal/my_lab/bfreeman/high_IO_destination/"
```

Required
Recommended
Optional

The flags are your resource requests and command to run is enclosed by `--wrap=""`

After you enter your `sbatch` command, SLURM will return..

```
Submitted batch job 29484165
```

This jobID is your way of tracking the job, controlling it, or obtaining info about it

Submitting jobs

The other is to create a SLURM script file using a recommended text editor:

- TextWranger/BBEdit on Mac
- GEdit/NotePad+ on PC
- nano, vi, emacs on Linux

The script files will contain resource requests (and other directives) and your code. And submit to SLURM via same `sbatch` command:

```
sbatch fastqc.slurm    #flags on sbatch line override in-script ones
```

OK, so we're going to get rather technical…

We will briefly highlight template SLURM script files for four types of jobs:

- *Single core (serial)*: sequentially-executing code that typically runs on one core
- *Multicore (multithreaded)*: code that is structured to allow multiple parts to run concurrently (in parallel) across multiple cores on one compute node
- *Multicore (openMP)*: a special type of multithreaded code
- *Multinode (MPI)*: code designed to run in parallel, but across multiple compute nodes and communicate with one another through a Message Passing Interface

Submitting Jobs - Single Core

`fastqc.slurm` file contents:

Required

```
#!/bin/bash
#SBATCH --open-mode=append        # ensure output files are not overwritten
#SBATCH -p serial_requeue         # Partition to submit to (comma separated)
```

Recommended

```
#SBATCH -J frog_fastqc            # Job name
#SBATCH -n 1                      # Number of cores
#SBATCH -N 1                      # Ensure that all cores are on one machine
#SBATCH -t 0-1:00                 # Runtime in D-HH:MM (or use minutes)
#SBATCH --mem 100                 # Memory in MB
#SBATCH -o fastqc_%j.out          # File to which standard out will be written
#SBATCH -e fastqc_%j.err          # File to which standard err will be written
```

Start

```
#SBATCH --mail-type=ALL           # Type of email notification: BEGIN,END,FAIL,ALL
#SBATCH --mail-user=rmf@123.com   # Email to which notifications will be sent
```

Required

```
source new-modules.sh; module load fastqc/1.0.0-fasrc01

cd my_output_directory
fastqc --casava -o fastqc_reports A01_R1.pair.fastq.gz
...
... do more processing here...
```


Submitting Jobs - Multicore

`bowtie.slurm` file contents:

Required

```
#!/bin/bash
#
#SBATCH -p serial_requeue,general # Partition to submit to (comma separated)
```

Recommended

```
#SBATCH -J frog_bowtie            # Job name
#SBATCH -n 8                      # Number of cores
#SBATCH -N 1                      # Ensure that all cores are on one machine
#SBATCH -t 0-6:00                 # Runtime in D-HH:MM (or use minutes)
#SBATCH --mem 8000                # Memory pool in MB for all cores
#SBATCH -o bowtie_%j.out          # File to which standard out will be written
#SBATCH -e bowtie_%j.err          # File to which standard err will be written
```

Start

```
#SBATCH --mail-type=ALL           # Type of email notification: BEGIN,END,FAIL,ALL
#SBATCH --mail-user=rmf0123.com   # Email to which notifications will be sent
```

Required

```
source new-modules.sh; module load bowtie/1.1.1-fasrc01

cd my_output_directory
bowtie -q -p $SLURM_NTASKS -1 A01_R1.pair.fastq.gz -2 A01_R1.pair.fastq.gz
...
... do more processing here...
```

Submitting Jobs - Multicore #2

`omp_test.slurm` file contents:

Required

```
#!/bin/bash
#
#SBATCH -p general                  # Partition
```

Recommended

```
#SBATCH -J omp_test                 # Job name
#SBATCH -n 8                        # Number of cores
#SBATCH -N 1                        # Make sure all cores are on a single node
#SBATCH -t 0-1:00                   # Runtime limit
#SBATCH --mem 8000                  # Memory pool in MB for all cores
#SBATCH -o omp_test_%j.out          # Standard output
#SBATCH -e omp_test_%j.err          # Run-time errors
```

Start

```
#SBATCH --mail-type=ALL             # Type of email notification
#SBATCH --mail-user=rmf@123.com     # Email to which notifications will be sent
```

Required

```
export OMP_NUM_THREADS=$SLURM_NTASKS # Specify number of OMP threads

source new-modules.sh; module load intel
./omp_itest.x
...
... do more processing here...
```

Submitting Jobs - Multinode

`mpi_test.slurm` file contents:

Required

```
#!/bin/bash
#
#SBATCH -p general                  # Partition
```

Recommended

```
#SBATCH -J mpi_test                 # Job name
#SBATCH -n 128                      # Number of cores
#SBATCH -N 2-10                     # # nodes min (-max optional) (-N param optional)
#SBATCH -t 0-1:00                   # Runtime limit
#SBATCH --mem-per-cpu=4000          # Memory in MB per core
#SBATCH -o mpi_test_%j.out          # Standard output
#SBATCH -e mpi_test_%j.err          # Run-time errors
```

Start

```
#SBATCH --mail-type=ALL             # Type of email notification
#SBATCH --mail-user=rmf@123.com     # Email to which notifications will be sent
```

Required

```
source new-modules.sh; module load intel
module load openmpi

mpirun -np $SLURM_NTASKS ./mpi_test.x
...
... do more processing here...
```

Controlling Jobs & Getting Job Info

`scancel` may become your best friend

```
scancel JOBID                                  # specific job
scancel -u bfreeman                            # ALL my jobs
scancel -u bfreeman -J many_blast_jobs         # named jobs
scancel -u bfreeman -p bigmem                  # ALL in partition
```

`squeue` gives info on currently running jobs

```
squeue -u bfreeman                             # jobs for bfreeman
squeue -u bfreeman --states=R | wc -l          # # of Running jobs
```

`sacct` gives current and historical information

```
sacct -u bfreeman                              # jobs for bfreeman
sacct -u bfreeman -p bigmem --starttime=9/1/14 # same+bigmem partition
sacct -j JOBID --format=JobID,JobName,ReqMem,MaxRSS,Elapsed # RAM requested & used!!
```

Check out Common SLURM Commands: http://fasrc.us/easyslurm

SLURM, LSF, SGE, PBS/Torque rosetta stone: http://fasrc.us/move2slurm

Basic Troubleshooting

Before seeking help, take some basic steps to ascertain what is going on with your job:

- Use `squeue` and `sacct` with `--format=` option to query details from SLURM
  - Are you having Fairshare issues (`Priority`)?
  - Is your job waiting for space (`Resources`)?
  - Will your job ever run (`Dependency`)?
  - Is there an error code or message
- Check your log files
  - You did specify both `-o` and `-e`, yes?
  - No log files? Does the path to your log files exist before the job start?
  - Message about `Pre-emption`, `Timeout`, or `Failure`?
  - The last error in the log is usually not the problem. The first one is!
- Did you request e-mail messages for your jobs with `--mail-type=`?
- Is your SLURM script formatted properly?
- Are you loading legacy modules? Possible software/library conflicts?

Check out out Tips@12 presentation http://fasrc.us/fasrcmaterials

Advanced Topics on Odyssey

HARVARD Faculty of Arts and Sciences RESEARCH COMPUTING

Not enough time to cover, but look on our website for...

- *FairShare*:
  - Assigned priority based on past job CPUTime usage and RAM request
  - Is shared among all lab members
  - Use sshare to query SLURM. Low priority < 0.5 < High Priority
- *Job dependencies*:
  - JobA & B submitted at the same time, but JobB starts when JobA has finished
  - Great for pipelines and complex workflows
- *Job arrays*:
  - Large bundle of jobs run individually but handled as one unit
  - Is more efficient and is kinder on the scheduler
- Pleasantly parallel jobs
- OpenMP (multicore) & MPI (multinode)
- Parallel IO, R, MATLAB, Python

Check out documentation at: http://fasrc.us/fasrcdocs

Example scripts at: http://fasrc.us/slurmutils

Problems, Pitfalls, and Prevention

HARVARD Faculty of Arts and Sciences RESEARCH COMPUTING

This is a shared resource, so everyone has skin in the game. And you can help us and yourself…

- Node and cluster problems are not unusual, esp. as large as system as Odyssey: I/O errors, node failures, memory errors, etc. Let us know if you see these.
- Review our Usage & Responsibilities guidelines: http://fasrc.us/hpccustoms
- Review our Common Pitfalls, lest you fall victim: http://fasrc.us/hpcpitfalls

Don't use multiple cores for R and Python scripts

These interpreters/runtime environments are can one use 1 core. Don't waste please.

PEND for >48 hrs

Asking for very large resource requests (cores/memory);very low Fairshare score

Quick run and FAIL...Not including -t parameter

no -t means shortest possible in all partitions == 10 min

Asking for multiple cores but forgetting to specify one node

-n 4 -N 1 is very different from -n 4

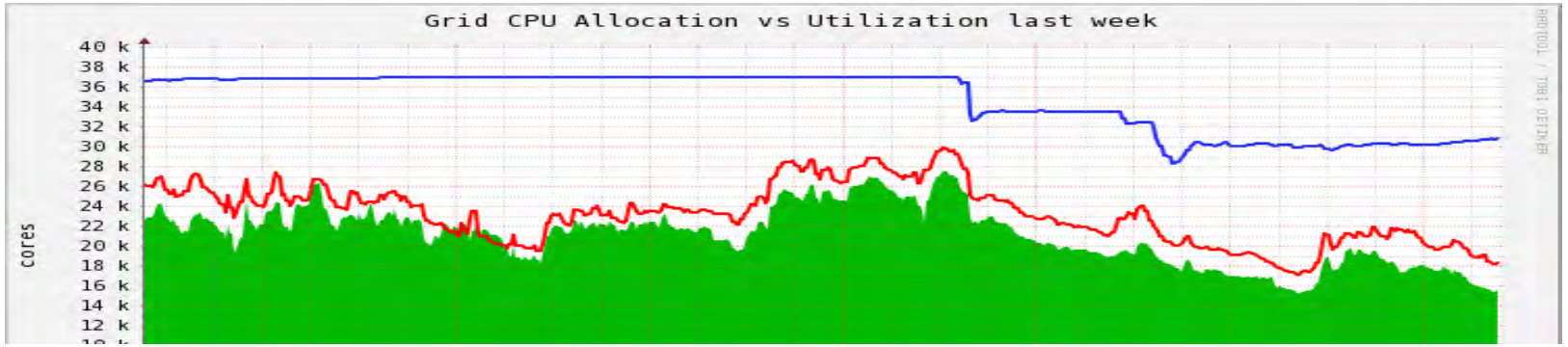
Not specifying enough cores

prog1 | prog2 | prog3 > outfile should run with 3 cores

Causing massive disk I/O on home folders/lab disk shares

your work & others on the same filesystem slows to a crawl; simple commands like ls take forever

Job efficiency



RC regularly reviews jobs based on their effective usage of their SLURM reservations (cores, memory, time, disk, ...) to promote maximum utilization of these resources.

- Over-requesting resources negatively effects the scheduling priority of your own jobs and blocks other users from these resources, which further lowers the overall research output for all HU users.
- Under-requesting resources negatively effects your job and those running on the same nodes; and potentially other jobs on the same filesystem

You may be contacted if you are regularly are having issues with your job efficiency and we will work with you to improve your performance.

Can calculate the efficiencies with the following formula:

```
sacct -u RCUSERNAME --format=user,state,jobid,alloccpus,elapsed,cputime
EffCPUs = CPUTime / Elapsed
%Eff = CPUTime / (AllocCPUs * Elapsed)
```

Getting Help

RC Website & Documentation -- only authoritative source
https://rc.fas.harvard.edu/

Submit a ticket on the portal https://portal.rc.fas.harvard.edu/

Best way to help us to help you? Give us...

Description of problem
Additional info (login/batch? partition? JobIDs?)
Steps to Reproduce (1., 2., 3...)
Actual results
Expected results

OdyBot, for quick-fix problems http://odybot.org/

Take-home Message…

If you can mind these Top 5 items, you'll be an Odyssey rock star!

1. Use the appropriate partition for your job
2. Don't run large numbers of jobs out of home or lab directories; use `/scratch` or `/n/regal` instead
3. Lower your RAM usage and use `--mem` where possible
4. Pass along to your code the number of cores you requested from SLURM (usually $SLURM_NTASKS) if using more then 1 core; and use `-N 1` unless you know what you're doing
5. Ensure your jobs run for at least 5 - 10 minutes and keep job counts in a reasonable range (≤ 1000)

Research Computing

Please talk to your peers, and …
We wish you success in your research!

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