

# Intermediate O2

## HMS Research Computing

We'll allow a few minutes for people to join the class.  
Slides are available at: [github.com/hmsrc/user-training](https://github.com/hmsrc/user-training)

Intermediate\_O2.pdf

HMS-RC help: [rchelp@hms.harvard.edu](mailto:rchelp@hms.harvard.edu)

# Course Objectives

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- Transferring data with rsync
- Linux tools
- Bash “for” loops
- Handling command output
- Customizing your O2 account environment
- More about SLURM
- Cron
- Q&A

# Housekeeping



- Please show your real first/last name in your Zoom profile so we can take attendance.
- This class is not being recorded.
  - Audio/Video for attendees is disabled by default.
- **Zoom Chat** anytime during class: for technical problems or general questions.
  - If it's not a quick answer, we should have time to discuss questions at the end of class.



# Resources

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- O2 docs:
  - [harvardmed.atlassian.net/wiki/spaces/O2](https://harvardmed.atlassian.net/wiki/spaces/O2)
  - [O2 portal](#) — O2's web interface!
- Research Computing Website
  - [it.hms.harvard.edu/rc](https://it.hms.harvard.edu/rc)
- Get Help:
  - [rchelp@hms.harvard.edu](mailto:rchelp@hms.harvard.edu)
- HMS RC Office Hours: Wed from 1-3pm via Zoom:
  - [rc.hms.harvard.edu/office-hours](https://rc.hms.harvard.edu/office-hours)

# Stay informed about O2

## O2 Status Page

- to view ongoing outages and scheduled maintenance
- <https://harvardmed.atlassian.net/wiki/spaces/O2/pages/1600651306/O2+Cluster+Status>
- (also linked from the main O2 wiki page)

## Twitter

For public-facing announcements

[twitter.com/hms\\_rc](https://twitter.com/hms_rc)

## o2-announce email list

- Required for all O2 users
- Service outages, scheduled maintenance, other news about O2

## Message of the Day (MOTD)

- That message in the terminal you see when you login to O2.

# O2, 2FA, and the HMS VPN

You can currently login to O2 without using VPN

- Duo (2FA) authentication is then required for each login

VPN can not support large file transfers

- Log out of VPN when copying large data between your desktop and O2, or any HMS filesystem (e.g. research.files.med.harvard.edu )
- HMS IT may kill any processes which are impacting VPN service.

# Login to O2

If you don't have an O2 account, we can assign you a temporary one for the class.



# O2 data transfer: which tool to use?

	Local	Remote	Not supported
Tools	cp rsync	sftp scp rsync wget ftp rclone [more]	<u>Inbound</u> FTP and generally anything which not sending over SSH (port 22).







# rsync: most common use

- Local on O2:

**\$** `rsync -av source/ destination/`

`-a (-rlptgoD , recursive and preserves permissions)`

`-v (verbose)`

- Over a network to O2 (*ssh option is required*):

**\$** `rsync -av -e ssh source/ user@transfer.rc.hms.harvard.edu:destination/`

`-z (data compression)` may be useful for external transfers

- Dry run (`-n`): test your command without actually copying data

**\$** `rsync -n -av source/ destination/`



# Exercise: rsync

- Copy the class directory with rsync: (*dry run: -n*)

```
$ rsync -n -av /n/groups/rc-training/o2_intermediate ~/
```

- For real:

```
$ rsync -av /n/groups/rc-training/o2_intermediate ~/
```

*Note that adding a trailing slash on the source directory will have rsync only copy the files within, not the directory itself.*



# rsync: more options

- Synchronize directories (be careful !!)

`$ rsync -delete -av source/ destination/`

- this **overwrites and deletes** files in the destination which don't match what is in the source.

- Set permissions

`$ rsync -chmod=ug+rw [..]`

- Exclude patterns or a list of files from transfer:

`$ rsync -exclude '*.bam' [..]`

`$ rsync -exclude-from 'exclude-list.txt' [..]`

# Globus: external data sharing

To share data from O2 to external collaborators

- provides secure access to individual folders on O2 for collaborators outside of Harvard / HMS.
- HMS credentials or O2 user accounts are not required for the collaborators when using Globus.
- See the [Globus documentation](#) on the O2 wiki for details
- HMS RC offers periodic information sessions about Globus

# Command line shortcuts

- Tab autocomplete filename / command
- Ctrl + c kill command you are currently running
- Ctrl + a move to the beginning of the line
- Ctrl + d logout
- Ctrl + e move to the end of the line
- Ctrl + k erase line to the right
- Ctrl + l clear the terminal
- Ctrl + u erase line to the left
- Ctrl + w erase word to the left
- [arrow keys] move cursor, browse command history

# head / tail / less / more / cat

- Commands to view text in a file or stream.
- Exercise: examine contents of a data file

```
$ cd ~/o2_intermediate/data
```

```
$ cat example.gtf
```

```
$ head example.gtf
```

```
$ head -20 example.gtf
```

```
$ tail example.gtf
```

```
$ tail -20 example.gtf
```

```
$ tail -f example.gtf (CTRL-C to quit)
```

```
$ more example.gtf ("q" or CTRL-C to quit, "return" or "space" to scroll)
```

```
$ less example.gtf ("q" to quit, arrows and other keys for navigation)
```

# ln

- A link is a special file type
  - `ln` with the `-s` option is the most common use: “symbolic”
  - Symbolic links work across filesystems
- Example / Exercise:
  - `$ mkdir work` (make a directory)
  - `$ ln -s work shortcut` (make a link called “shortcut”)
  - `$ ls -l` (lower-case “L” file type)

# find

- `find [path to search] [expression] [actions]`
  - `-name` : the filename / pattern
  - `-user` : user owner
  - `-group` : group owner
  - `-type` : type of file (plain file, directory, pipe. etc)
  - `-ctime` : time of file creation
  - `-atime` : last access time of a file
  - `-mtime` : last modification time of a file
  - `-exec [command]` : runs a command against find's output



# find: examples

- List all files matching the name \*.bam

```
$ find ./dir -name '*.bam'
```

- Make all files group-writable under a directory:

```
$ find ./dir -type d -exec chmod -v g+rwxs {} \;
```

```
$ find ./dir -type f -exec chmod -v g+rw {} \;
```

```
$ find ./dir -exec chgrp -v labgroup {} \;
```

- Remove files not updated in the past 60 days:

```
$ find ./dir -mtime +60d -exec rm -v {} \;
```

# find: exercise

- Create symbolic links to all bam files located under a directory tree:

```
$ cd ~/o2_intermediate
```

```
$ find . -name '*.bam'
```

```
$ find . -name '*.bam' -exec ln -s {} \;
```

```
$ ls -l
```

- Don't delete these links – we'll use them later!

# WC

- word count
  - `-l` print number of lines
  - `-w` print number of words
- Example: (how many lines are in a file)

```
$ cd ~/o2_intermediate/data
```

```
$ wc -l example.gtf
```

# du

- estimate file space usage
  - [default] print summary size only (Kb)
  - -a print usage of all files
  - -h print human readable format (Kb/Mb/Gb/Tb)
- Example: (how many lines are in a file)

```
$ cd ~/o2_intermediate/data
```

```
$ du -h example.gtf
```

```
$ du -a
```

```
$ du -ah
```

# Commands for Text Processing



# sort

- sort lines of text

```
$ sort file.txt
```

- -r (reverse order)
- -f (ignore case)
- -h (human numeric sort: e.g. 2K, 1G, 500M)
- -u (remove duplicate lines)

# Exercise: sort

```
$ cd ~/o2_intermediate
```

```
$ cat sort.txt
```

```
$ sort sort.txt
```

```
$ sort -r sort.txt
```

# uniq

- report or omit repeated lines

```
$ uniq file.txt
```

- -i (ignore case)
- -c (prefix lines by number of occurrences)
- -d (print only repeated lines)
- -u (print only unique lines)



# Exercise: uniq

Try these commands:

```
$ cd ~/o2_intermediate
```

```
$ cat uniq.txt
```

```
$ uniq uniq.txt
```

(remove duplicate entries)

```
$ uniq -d uniq.txt
```

(show duplicates only)

```
$ uniq -u uniq.txt
```

(show unique entries only)

```
$ uniq -c uniq.txt
```

(unique entries with count)

# grep (global regular expression print)

- print lines matching a pattern
  - `$ grep pattern file.txt`
  - `$ grep '#pattern 2' file.txt`
- a few common options:
  - `-i` (case-insensitive)
  - `-v` (does not match the pattern)
  - `-n` (precede matching line with a line number)

# Exercise: grep

```
$ cd ~/o2_intermediate/data
```

```
$ grep stop_codon example.gtf
```

```
$ grep -v stop_codon example.gtf
```

```
$ grep -n stop_codon example.gtf
```

```
$ grep -i cds example.gtf
```

# cut

- remove sections from each line in a file / stream
  - **-d** defines delimiter (default is a Tab)
  - **-s** prints only lines containing a delimiter
  - **-f** prints specified fields
- Examples:
  - `$ cut -f 1 file.txt` (print 1st field only)
  - `$ cut -f 1,3 file.txt` (print 1st & 3rd fields)
  - `$ cut -s -d ":" -f 1 file.txt` (colon space delimiter)
  - `$ O2squeue | cut -s -d " " -f 1` (list of O2 job IDs)

# Exercise: cut

- remove sections from each line in a file / stream
- default delimiter is a Tab

```
$ cd ~/o2_intermediate/data
```

```
$ head example.tab
```

```
$ cut -f 1,2 example.tab | head
```

```
$ cut -f 3,4 example.tab | head
```

# paste

- Write lines consisting of the sequentially corresponding lines from each FILE, separated by TABs, to standard output.
- **-d** defines delimiter (default is a Tab)
- Examples:
  - \$ paste file1.txt file2.txt
  - \$ paste file1.txt file2.txt > out.tsv (tab separated file)
  - \$ paste -d , file1.txt file2.txt > out.csv (comma separated file)

# Working with Command Output



# Command output redirection:

- Redirect: **>**
  - sends output to a file, overwrites any existing file  
`$ grep pattern file.txt > out.txt`
- Append: **>>**
  - sends output to a file, appends to any existing file  
`$ grep pattern file.txt >> out.txt`
- Pipe: **|**
  - sends output to be input for another application  
`$ cut -1 file.txt | sort | uniq -c`



# Exercise: handling command output

- Sort field entries from a data file ([example.gtf](#))
- default delimiter is a Tab

```
$ cd ~/o2_intermediate/data
```

```
$ cut -f 4 example.gtf > out.txt
```

```
$ grep -i cds example.gtf >> out.txt
```

```
$ cut -f 4 example.gtf > out.txt
```

```
$ cut -f 4 example.gtf | sort -n | uniq -c
```

```
$ grep stop_codon example.gtf | wc -l
```

# Redirecting Standard Error (stderr)

- **bash syntax:**

<code>\$ command 2&gt;out.err</code>	(send stderr to a file)
<code>\$ command 2&gt;&amp;1</code>	(send stderr to stdout)
<code>\$ command &gt; out.txt 2&gt;&amp;1</code>	(send stderr and stdout to a file)

- **Exercise:**

<code>\$ cd ~/o2_intermediate</code>	
<code>\$ cat no.txt</code>	(file does not exist — error)
<code>\$ cat no.txt 2&gt;out.err</code>	(saves stderr to a file: <code>out.err</code> )

# Customizing your O2 account



# Customizing your O2 account

- Aliases: create your own commands!

```
$ alias h=history
```

- Change your default umask

- Example: create group-writable files by default:

```
$ umask 0002
```

- Set, environment variables like command path:

```
$ export PATH=$PATH:/home/user/bin
```

# Adding customizations on login

- For the bash shell (default on O2):
  - **~/.bash\_profile**
    - executed on login
    - executed once before you get a prompt.
  - **~/.bashrc**
    - Supplemental config file, executed each time you run “bash”
    - On O2, gets run from ~/.bash\_profile
    - Typically, this is where most customizations go:
    - **aliases, modules, \$PATH, other variables, etc.**

# Sample ~/.bashrc file

```
$ cat ~/.bashrc
```

```
#
```

```
alias h history
```

```
#
```

```
module load gcc/6.2.0
```

```
module load R/4.1.1
```

```
#
```

```
export PATH=$PATH:/home/user/bin
```

```
export DUO_PASSCODE=push
```

# Exercise: edit your .bashrc file

```
$ nano ~/.bashrc
```

(Add some things you would like to set automatically on login)

```
$ source ~/.bashrc
```

(to manually run it without having to re-login)

Try it out! (Run an alias command, etc)

# bash “for” loops





# Automate commands with a “for” loop

- Repeat commands against an designated list
  - this syntax is for **bash**, but other shells (tcsh) are different
- Examples
  - `$ for i in 1 2 3 ; do mkdir $i ; done`
  - `$ for i in `cat list` ; do cp $i ~/work ; done`
  - more complex loops can be put in bash scripts
  - also useful for submitting batches of jobs to O2!

# “for” loop in a shell script

```
#!/bin/bash
```

```
list=/home/user/files.txt
```

```
for i in `cat $list`
```

```
do
```

```
    [command 1]
```

```
    [command 2]
```

```
done
```

# more about Slurm...



# Job Monitoring

---

```
$ O2squeue  
$ squeue -u your_user  
$ squeue -u your_user -t PENDING  
$ squeue -u your_user -t RUNNING  
$ squeue -u your_user -p short  
$ scontrol show jobid <jobid>  
    (for more details)  
  
$ O2sacct  
$ sacct -j <jobid>
```

# Jobs with command line arguments

(example: arguments.sbatch)

---

```
#!/bin/bash
```

```
#SBATCH -p short    #partition
```

```
#SBATCH -t 0-01:00 #time days-hr:min
```

```
#SBATCH -o %j.out   #out file
```

```
#SBATCH -e %j.err   #error file
```

```
echo $1
```

# Jobs with command line arguments

---

- Run the following:

```
$ cd ~/o2_intermediate
```

```
$ sbatch arguments.sbatch hello
```

```
$ O2squeue (to view job status)
```

- The output file will contain the argument “hello”
- This technique gets more useful when submitting from a script and the arguments vary over iterations.

# A better example (bamsort.sbatch)

---

```
#!/bin/bash
#SBATCH -p priority #partition
#SBATCH -t 0-01:00  #time days-hr:min
#SBATCH -o %j.out   #out file
#SBATCH -e %j.err   #error file

module load gcc/6.2.0
module load samtools

samtools sort $1 > "${1%.*}.sorted.bam
#where $1 is a bam data file
```

# Using sbatch with a bash “for” loop

- To submit a bunch of separate jobs systematically:

```
$ for i in [input] ; do [sbatch command] ; done
```

- Exercise (remember those symbolic links?):

```
$ cd ~/o2_intermediate
```

```
$ for i in *.bam ; do sbatch bamsort.sbatch $i ; done
```

```
$ ls -l *.sorted.bam           (to list the output files)
```



# Canceling one or more job

---

The [-u] option is always required.

```
$ scancel -u your_user
```

```
$ scancel -u your_user -v[vv]
```

```
$ scancel -u your_user -p short
```

```
$ scancel -u your_user -t PENDING
```

```
$ scancel -u your_user -t RUNNING
```

```
$ scancel -u your_user -t SUSPENDED
```

```
$ scancel -u your_user JOBID1 JOBID2 [..]
```

# Cron



# Process automation: cron



- Task Scheduler for Linux
- O2 has a centralized cron server where jobs get executed.
- Examples:
  - Automate a nightly rsync process
  - Run a weekly analysis report
  - Purge old files on a schedule



# Cron: Editing a Crontab

- Create/Edit a crontab from a login server using: **crontab -e**
- Format of a cron job process:

[Minute] [Hour] [Date] [Month] [Day of the Week] Command

Asterisk (\*) = “every”

- Example: have a job run at 2:00am every Monday:

```
0 2 * * 1 sbatch /home/user/rsync.sbatch
```

# Thank you!

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- The Harvard Training Portal will be emailing you a short survey about the class. Please complete it so we can learn what works, what needs improvement, and what you'd like to see offered in the future!