

Intermediate O2

HMS Research Computing



Course Objectives

- Transferring data with rsync
- Linux tools
- Bash “for” loops
- Handling command output
- Customizing your O2 account environment
- SLURM deeper dive
- Cron
- Slides online at: github.com/hmsrc/user-training
 - **IntermediateO2_Spring2019.pdf**

Login to O2



Linux tools

Commands	File Searching	Process Management	Editing Text Files
Show current directory Change to directory <i>dir</i> Create a new directory <i>dir</i> Delete directory <i>dir</i> List contents directory <i>dir</i>	Search for <i>pattern</i> in <i>file</i> Search for <i>pattern</i> in all files Invert search Recursive search Multiprocess search Locate <i>file</i> Which <i>cmd</i> Find <i>dir</i> -name <i>pattern</i> Find <i>file</i> in <i>dir</i>	Show processes of user Show all processes Show all processes in detail Show processes in real-time Run command in background Kill currently active process Kill currently active process Kill suspended process in background Kill background process to foreground Kill with process id <i>pid</i> Kill (ungraceful)	nano Text editor Shortcuts Ctrl-o Save file Ctrl-x Close file Ctrl-r Open file Ctrl-k Cut line of text Ctrl-u Paste line of text Ctrl-d Delete character Ctrl-w Search for text
File Options	Standard IO Streams	Text File Operations	GUI applications via Command
-a all inc. hidden -l long format -t sort by time -S sort by size -r reverse order -R recursive	stdin Input typed on terminal stdout Output on the terminal stderr Errors output to terminal echo <i>string</i> Write <i>string</i> to stdout	wc Line and character count sort <i>file</i> Sort uniq <i>file</i> Display lines sed 's/abc/def/g' <i>file</i> Replace cut -d " " -f <i>N</i> <i>file</i> Display cut -d " " -f <i>N-N</i> <i>file</i> Display	gedit Text editor Wireshark Packet capture and analysis eog Image viewer xpdf PDF viewer nautilus File explorer
File Manipulation	Redirection	Pipes and Filters	Administrator Privileges
Create file <i>file</i> Copy <i>file1</i> to <i>file2</i> Move <i>file1</i> to <i>file2</i> Delete <i>file</i> Display contents of <i>file</i> Concatenate files Display <i>file</i> (paginated), q to quit Show first 10 lines Show last 10 lines -n <i>N</i> <i>N</i> lines -f Continuous update	<i>cmd</i> > <i>file</i> <i>cmd</i> < <i>file</i> <i>cmd</i> >> <i>file</i> <i>cmd</i> 2> <i>file</i> <i>cmd</i> &> <i>file</i>	<i>cmd1</i> <i>cmd2</i> <i>cmd1</i> & <i>cmd2</i>	sudo <i>cmd</i> Execute <i>cmd</i> with superuser privileges su <i>username</i> Switch to user <i>username</i>

Command line shortcuts

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

O2 data transfer: which tool to use?

	Local	Remote	Not supported
Tools	cp rsync	sftp scp rsync wget ftp [more]	<u>Inbound</u> FTP and anything else which does not transmit 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:

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

`-z (data compression) option may be useful`

- Dry run: test your command without actually copying

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



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' [..]`



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 ~/
```

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
```

```
$ less example.gtf
```

```
$ more example.gtf
```

```
$ head example.gtf
```

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

```
$ tail example.gtf
```

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

```
$ tail -f example.gtf
```

(CTRL-C to quit)

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
 - *(and lots more...)*

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 {} \;
```

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
```

- a few common options:
 - -r (reverse order)
 - -h (human numeric sort: e.g. 2K, 1G, 500M)
 - -u (remove duplicate lines)

Exercise: sort

```
$ cd ~/o2_intermediate
```

```
$ sort sort.txt
```

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

uniq

- report or omit repeated lines

```
$ uniq file.txt
```

- with no options, `uniq` prints all lines but removes duplicate entries
- a few common options:
 - `-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
```

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

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

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

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
```

```
$ cut -f 1,3 example.tab
```

awk and sed

- awk

- a special-purpose programming language for text processing
- Does similar things as PERL, but sometimes awk gets it done quicker.
- Example: calculate the average of column 2:

```
$ awk '{x+=2}END{print x/NR}' file.txt
```

- sed

- a stream editor that works on a per-line basis.
- Example: global substitution of the string “Harvard” -> “HMS”

```
$ sed 's/Harvard/HMS/g' doc.txt > doc_new.txt
```

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
```

```
$ 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>out.err</code>	(send stderr to a file)
<code>\$ command 2>&1</code>	(send stderr to stdout)
<code>\$ command > out.txt 2>&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 >out.err</code>	(saves stderr to a new file)

Customizing your O2 account



Customizing your O2 account

- Aliases: create your own commands!

```
$ alias ll='ls -la'
```

```
$ 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

- `~/.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 ll 'ls -la'
```

```
alias h history
```

```
#
```

```
module load gcc/6.2.0
```

```
module load R/3.5.1
```

```
#
```

```
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 $x ; done`
 - `$ for i in `cat list` ; do cp $x ~/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
```

a few things about Slurm...



Jobs with command line arguments

```
#!/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
```


Exercise: Jobs with arguments

- Run the following:

```
$ cd ~/o2_intermediate
```

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

- 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 short    #partition
#SBATCH -t 0-01:00  #time days-hr:min
#SBATCH -o %j.out    #out file
#SBATCH -e %j.err    #error file

## Update path for your account:
## dir=/home/rc_training000/o2_intermediate/data

module load gcc/6.2.0
module load samtools/1.9

samtools sort $1 > $dir/"${1%.*}".sorted.bam
#where $1 is a bam 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:

```
$ cd ~/o2_intermediate
```

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

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 [..]
```

Canceling jobs: exercise

```
$ cd ~/o2_intermediate
```

```
#submit some jobs and kill them:
```

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

```
$ scancel -u your_user      #kill all jobs
```

```
#repeat:
```

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

```
$ scancel -u your_user JOBID1 JOBID2
```

Job Monitoring

\$ 02squeue

\$ squeue -u your_user

\$ squeue -u your_user -t PENDING

\$ squeue -u your_user -t RUNNING

\$ squeue -u your_user -p short

\$ 02sacct

\$ sacct -j JOBID

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
```

For more direction

- <http://hmsrc.me/O2docs>
- <http://rc.hms.harvard.edu>
- RC Office Hours: Wed 1-3p Gordon Hall 500
- rchelp@hms.harvard.edu