High Performance Research Computing

A Resource for Research and Discovery



HPRC Short Course

Introduction to UNIX





For More Help...

Website: hprc.tamu.edu

Email: help@hprc.tamu.edu

Telephone: (979) 845-0219

Visit us in person: Henderson Hall, Room 114A

Help us, help you -- we need more info

- Which Cluster
- UserID/NetID
- Job id(s) if any
- Location of your jobfile, input/output files
- Application used if any
- Module(s) loaded if any
- Error messages
- •Steps you have taken, so we can reproduce the problem

Logging in to the system

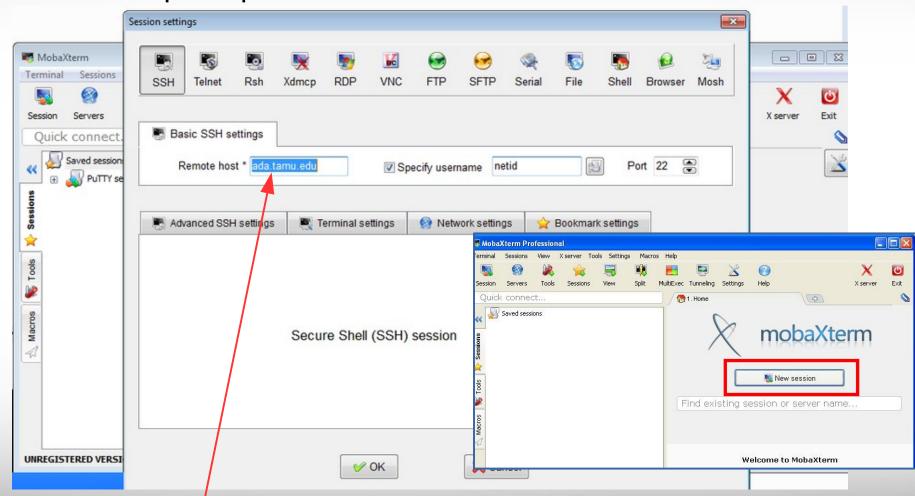
- SSH (secure shell)
 - The only program allowed for remote access; encrypted communication; freely available for Linux/Unix and Mac OS X hosts;
- For Microsoft Windows PCs, use MobaXterm
 - https://hprc.tamu.edu/wiki/HPRC:MobaXterm
 - You are able to view images and use GUI applications with MobaXterm
 - or *Putty*
 - https://hprc.tamu.edu/wiki/HPRC:Access#Using_PuTTY
 - You can not view images or use GUI applications with PuTTY

Your Login Password

- Both state of Texas law and TAMU regulations prohibit the sharing and/or illegal use of computer passwords and accounts;
- Don't write down passwords;
- Don't choose easy to guess/crack passwords;
- Change passwords frequently

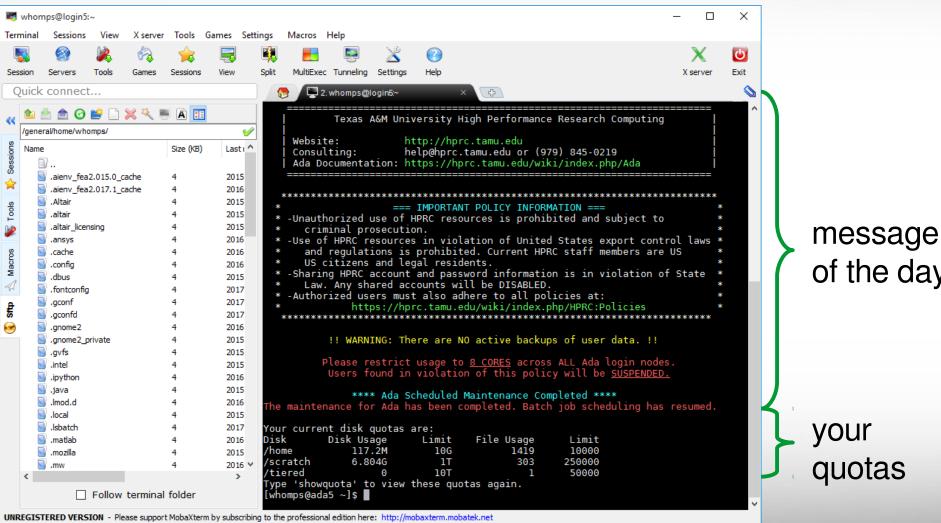
Using SSH - MobaXterm (on Windows)

https://hprc.tamu.edu/wiki/HPRC:MobaXterm



Use ada.tamu.edu as Remote host name.

Using SSH - MobaXterm (on Windows)



of the day

Using SSH (on a Linux/Unix Client)

https://hprc.tamu.edu/wiki/Ada:Access

You may see something like the following the first time you connect to the remote machine from your local machine:

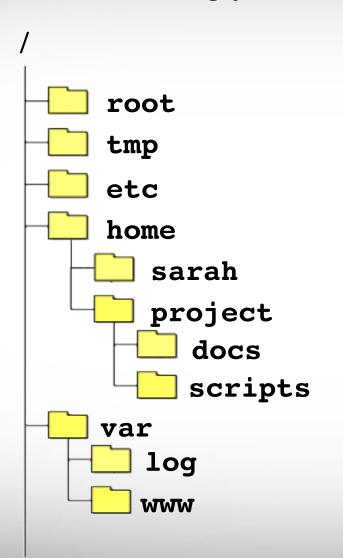
ssh user NetID@ada.tamu.edu

Host key not found from the list of known hosts. Are you sure you want to continue connecting (yes/no)?

Type yes, hit enter and you will then see the following:

Host 'ada.tamu.edu' added to the list of known hosts. user_NetID@ada.tamu.edu's password:

Finding your way around the UNIX directory structure



```
/root
/tmp
/etc
/home
/home/sarah
/home/project
/home/project/docs
/home/project/scripts
/var
/var/log
/var/www
```

Where Am I?

pwd command (print current/working directory)

UNIX commands in green

pwd

output in blue

/home/user NetID

UNIX Commands Have Options

Leave a space between the command and the options

double dash means there is a single option which is usually a descriptive word

--all show all files including hidden files which begin with .

single dash means each character is an option

- -a show all files including hidden
- -1 show file details

most options can be combined behind one dash

- -a show all files including hidden
- -1 show file details

current working directory back one directory

Search for UNIX Commands Options

Search the manual page for the UNIX command 1s

man 1s

Page up Page down Spacebar Mouse scroll wheel

Move up one page Move down one page Move down one page Move up and down

/all
n
N
g
G

search the man page for the text 'all' search forward for next found match search backwards next found match go to first line Go to last line quit

File and directory names

```
Commonly used:
A-Z
a-z
0-9
.
dash
underscore
```

```
Avoid using:
     spaces
     parenthesis
()
     quotes
     Question mark
$
     Dollar sign
     Asterisk
     back slash
     forward slash
     colon
```

- Avoid spaces.
- File and directory names are case sensitive
- Avoid spaces in the file name ("my data file" vs "my_data_file.txt").

Common Directory Commands

• *mkdir* command to make a new directory:

```
mkdir directory name
```

• cd to change to another directory:

```
cd directory name
```

• **rmdir** to remove an empty directory:

```
rmdir directory name
```

Changing Directories: the cd cmd

To switch to the parent directory of the current directory:

```
cd ..
```

Return to home directory

```
cd
cd ~
cd ~/
```

Exercise:

```
cd
mkdir temp
mkdir temp/hg19
cd temp
pwd
cd hg19
pwd
```

See directory structure

```
tree
```

```
cd ../..

pwd

cd -

return to previous pwd

cd ...

pwd

cd

pwd

tree
```

Absolute vs. Relative Pathname

```
/root
/tmp
/etc
/home
/home/sarah
/home/sarah/project
/home/sarah/docs/README
/var
/var/log
/var/www
```

If you are in the project directory

```
pwd
/home/sarah/project
```

The relative path to the README file is ../docs/README

```
ls ../docs/README
```

The absolute path to the README file /home/sarah/docs/README

```
1s /home/sarah/docs/README
```

gedit text editor

From the UNIX terminal command line enter this command to start gedit and edit a file called my_favorite_foods.txt

the & will detach gedit from the terminal so you can continue to use the terminal

Naming files:

use all lower case characters separate words with an underscore make the file name very descriptive of what is in the file even if its rather long common file extensions:

- .pl a Perl script
 .py a Python script
- .gz a file that has been compressed (zipped) to reduce file size (.zip)
- .txt a generic text file
- .tsv tab separated values (columns are separated by a tab)
- .csv comma separated values
- .jar a Java ARchive file
- .png image file in png format
- .tar.gz compressed tar file (sometimes .tgz)



Use the tab key to complete a file name

Type the first few characters of the file name

then hit the tab key to auto complete the file name

```
ls -1 my_favorite_foods.txt
```

then hit enter to see the command results which will show the file size in human readable format

If the tab key did not complete the file name then either the file does not exist or there are two or more files that begin with the same characters in which case you need to hit tab twice then type a few more characters and hit tab again to complete.

Count lines in a file

wc my favorite foods.txt

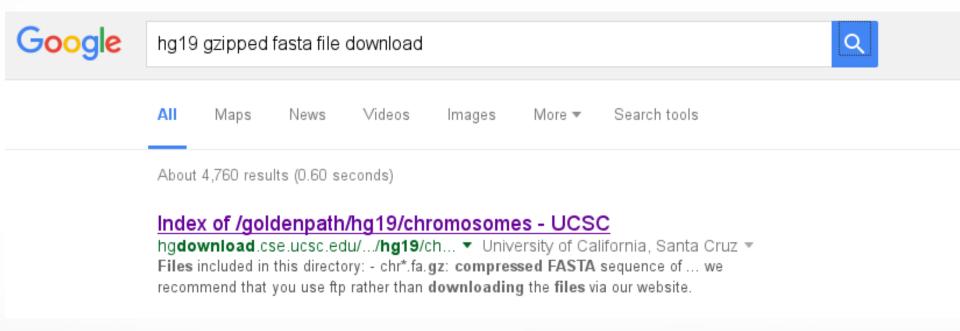
29 109 876 my favorite foods.txt

What does the output mean?

Use the man page for wc to find out.

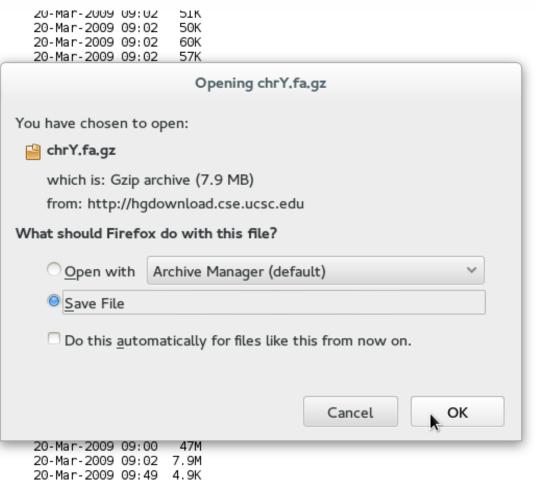
How do you just print the newline counts?

Download a File from the Web to your pwd

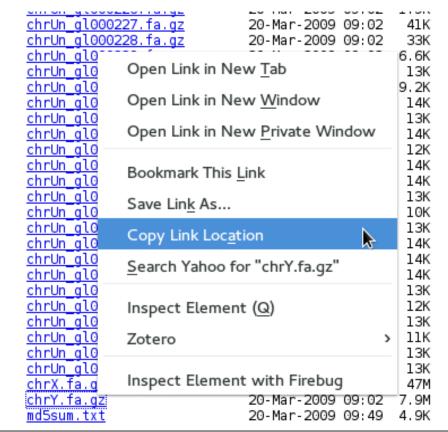


Don't Left Click and download a file to your desktop

cnrun qluuuzzu.ta.qz chrUn ql000221.fa.qz chrUn ql000222.fa.qz chrUn gl000223.fa.gz chrUn ql000224.fa.qz chrUn ql000225.fa.qz chrUn ql000226.fa.qz chrUn ql000227.fa.qz chrUn ql000228.fa.qz chrUn ql000229.fa.qz chrUn_ql000230.fa.qz chrUn ql000231.fa.qz chrUn ql000232.fa.qz chrUn_gl000233.fa.gz chrUn ql000234.fa.qz chrUn_gl000235.fa.gz chrUn ql000236.fa.qz chrUn ql000237.fa.qz chrUn ql000238.fa.qz chrUn ql000239.fa.qz chrUn ql000240.fa.qz chrUn gl000241.fa.gz chrUn ql000242.fa.qz chrUn ql000243.fa.qz chrUn ql000244.fa.qz chrUn gl000245.fa.gz chrUn ql000246.fa.qz chrUn ql000247.fa.qz chrUn gl000248.fa.gz chrUn ql000249.fa.qz chrX.fa.gz chrY.fa.dz md5sum.txt



Right Click and Copy the URL so you can download it directly to your UNIX computer



Copy a file directly to your UNIX directory

Use the wget command to get a file from a URL

Type wget then a space then click the middle mouse button to paste the URL (you can also use 'Shift + Insert' to paste into the UNIX terminal)

cd ~/temp/hg19

wget http://hgdownload.cse.ucsc.edu/goldenpath/hg19/chromosomes/chrY.fa.gz

wget http://hgdownload.cse.ucsc.edu/goldenpath/hg19/chromosomes/md5sum.txt

List the directory contents to see the file with details (-I) and human readable file sizes (-h)

ls -lh

Copying and renaming Files

Use the tab key to help prevent typos when typing filenames and directories

1a. cp ch (then hit tab)

UNIX will complete the file name for you

1b. cp chrY.fa.gz

Make a copy of the chrY.fa.gz file called chrY_copy.fa.gz

1c. cp chry.fa.gz chry_copy.fa.gz

Rename the chrY_copy.fa.gz file to chrY_hg19.fa.gz

mv chrY_copy.fa.gz chrY_hg19.fa.gz

Deleting Files: the *rm* cmd

```
rm [options] [file_name]
```

- Commonly used options
 - -i prompt user before any deletion

Use the wildcard * to list all files ending with gz

```
Exercise:
            rm -i chrY.fa.gz
```

Displaying File Contents

Check the file size before attempting to open with a text editor

```
ls -lh md5sum.txt
cat md5sum.txt
```

- cat prints all the contents of a file(s) to the screen.
- The **more** command, and its improved version **less**, display an text file one page at a time.
 - Hit space bar for next page
 - Type **q** to quit
 - Use **zmore** or **zless** for compressed files (.gz)

```
more md5sum.txt
less md5sum.txt
zmore chrY hg19.fa.gz
```

Displaying File Contents

 Use head and tail commands to see first and last 10 lines of a file respectively

```
head md5sum.txt
tail md5sum.txt
```

- **head** and **tail** are not for compressed files (.gz)
- There is not a zhead or ztail command
- Use zcat together with the head or tail command

```
zcat chrY hg19.fa.gz | head
zcat chrY hg19.fa.gz | tail
```

'grep' - Search pattern(s) in files

```
grep [options] PATTERN [files ...]
     grep chrX md5sum.txt
Count the number of lines that match pattern
    grep -c random md5sum.txt
Search multiple matches
     grep -e chrX -e chrY md5sum.txt
Exclude a pattern; show non-matching lines
     grep -v random md5sum.txt
Use zgrep for compressed files (.qz)
     zgrep chr chrY hg19.fa.gz
```



Piping output of UNIX commands

Use the pipe character | to send results to another command

Search the output of md5sum.txt for the string 'chrX'

```
cat md5sum.txt | grep chrX
```

Use the standard output redirect operator > to create a new file

```
grep chrX md5sum.txt > chr_xy.txt
```

Use the standard output redirect operator >> to append to a file

```
grep chrY md5sum.txt >> chr_xy.txt
```

History of your commands

- Your commands are saved to a file in your home directory (.bash_history)
- You can use the up/down arrows to scroll through your previous commands
- Type history to see all your commands

```
history | tail
```

See last 10 commands

Search your history commands using | and grep

```
history | grep wget
```

Types of File: the file cmd

```
file [name]
```

 Displays a brief description of the contents or other type information for a file or related object.

```
file md5sum.txt

md5sum.txt: ASCII English text
```

```
file chrY_hg19.fa.gz
```

```
chrY_hg19.fa.gz: gzip compressed data,
was "chrY.fa", last modified ...
```

CRLF line terminators

 Windows editors such as Notepad will add hidden return/line feed characters that can cause problems with some applications

```
file my file.txt
my file.txt: ASCII English text, with CRLF line terminators
 dos2unix my file.txt
 file my file.txt
my file.txt: ASCII English text
```

Editing an ASCII file

- There are many editors available under Linux.
- Text mode
 - nano (simple)
 - vi or vim (more advanced)
 - emacs (more advanced)
- Graphic mode (require X11)
 - gedit
 - xemacs / gvim
- Be aware of text file edited under Windows (CR/LF vs LF).
 Use dos2unix to convert a DOS/Windows edited text file to UNIX format.

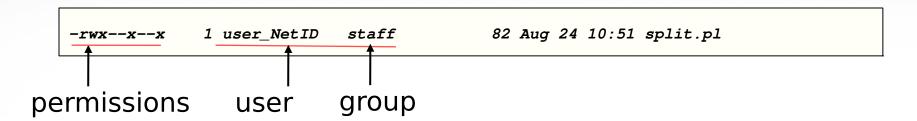
```
dos2unix my_dos_file.txt
```

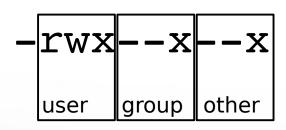
The UNIX Filesystem

File Attributes: A look with 1s

```
[user_NetID@ada ~]$ ls -1
total 37216
             7 user NetID
                            user NetID
                                              121 Sep 9 10:41 abaqus_files
drwx----
                                             2252 Aug 24 10:47 fluent-unique.txt
             1 user NetID
                            user NetID
                                          13393007 Aug 24 10:40 fluent-use1.txt
             1 user NetID
                            user NetID
             1 user NetID
                            user NetID
                                               533 Aug 24 11:23 fluent.users
drwxr-xr-x
             3 user NetID
                            user NetID
                                               17 May
                                                       7 16:56 man
             1 user NetID
                            user NetID
                                          24627200 Sep 9 10:49 myHomeDir.tar
                                      21 May 28 16:11 README -> /usr/local/etc/README
             1 root
lrwxrwxrwx
                       root
                                               162 Sep 7 12:20 spiros-ex1.bash
             1 user NetID
                            user NetID
             1 user NetID
                            user NetID
                                               82 Aug 24 10:51 split.pl
-rwx--x--x
             2 user NetID
                            user NetID
                                                6 May 5 11:32 verifyOLD
drwxr-xr-x
                                                                    file name
                                   group name
                      user name
                                                              file modification tim
                hard link count
                                                       file modification date
                                                   file size in bytes
       file permissions
```

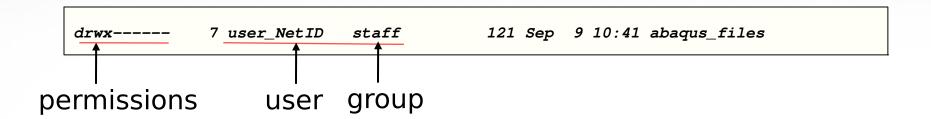
File Ownership and Permissions





- There are 3 sets of permissions for each file
 - 1st set user (the owner)
 - 2nd set group (to which file owner belongs)
 - 3rd set other (all other users)
- The r indicates read permission
- The w indicated write permission
- The x indicated execute permission

Directory Permissions



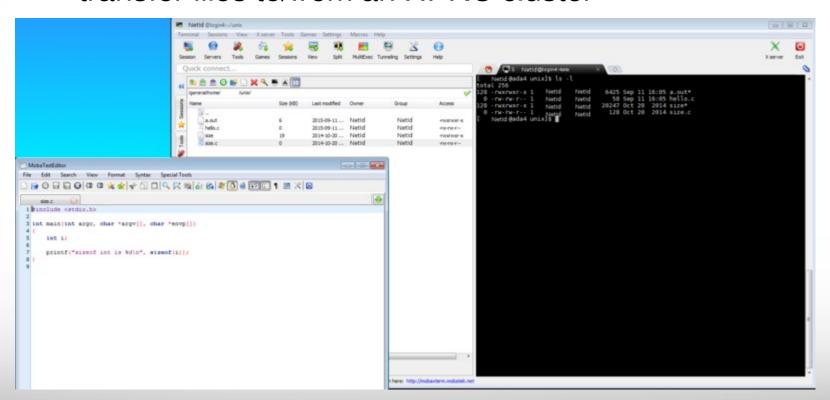
- The meanings of the permission bits for a directory are slightly different than for regular files:
 - r permission means the user can list the directory's contents
 - w permission means the user can add or delete files from the directory
 - x permission means the user can cd into the directory; it also means the user can execute programs stored in it
- Notice that if the file is a directory, the leading bit before the permissions is set to d, indicating directory.

Changing Attributes: the chmod cmd

chmod [options] [permission mode] [target_file]

Transfer data between Windows hosts with MobaXterm

 On a Windows system, you can use MobaXterm to transfer files to/from an HPRC cluster

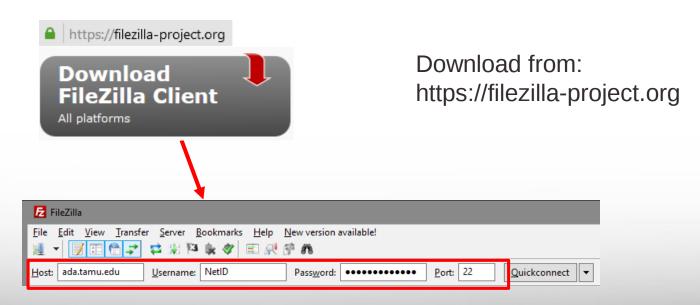


https://hprc.tamu.edu/wiki/HPRC:MobaXterm

File Transfers Using FileZilla

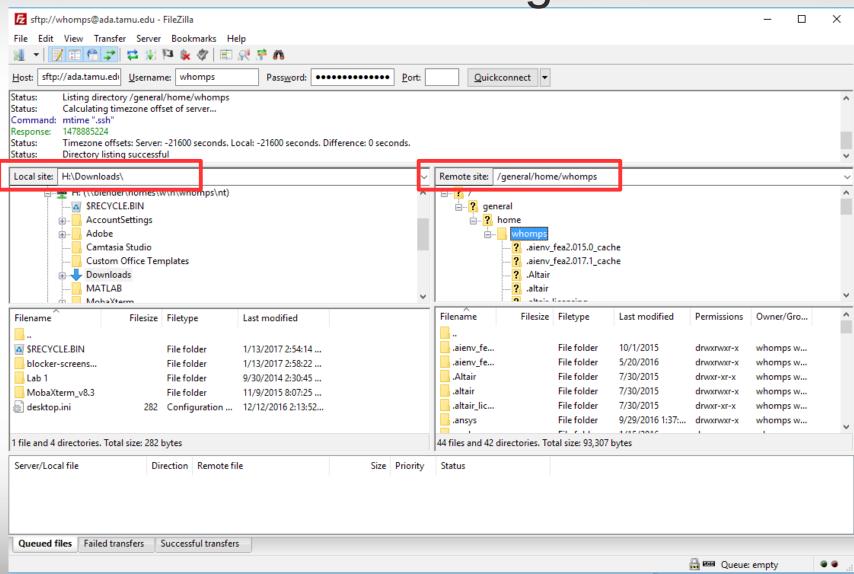
The FileZilla Client:

- 1) Available on Windows, OS X, and UNIX/Linux
- Allows permissions to be preserved or implied
- 3) Easy to use without previous experience
- 4) Can drag and drop files between computers



Connect with remote login

File Transfers Using FileZilla



Transfer data between UNIX hosts with scp

```
scp [[user@]host1:]filename1 [[user@]host2:]filename2
Copy a file from your UNIX desktop to your ada home directory
scp myfile1 user@ada.tamu.edu:
Copy & rename file from your UNIX desktop to dirl in your $HOME
scp myfile1 user@ada.tamu.edu:dir1/remote myfile1
Copy a file to your UNIX desktop from your ada home directory
scp user@ada.tamu.edu:myfile2 ./
scp user@ada.tamu.edu:myfile2 local myfile2
scp -r user@ada.tamu.edu:dir3 local dir/
```

Bash Environment Variables

HOME pathname of current user's home directory

PATH

the search path for commands. It is a colon separated list of directories in which the shell looks for commands.

SCRATCH pathname of current user's scratch directory

```
echo $HOME
/home/user NetID
echo $SCRATCH
/scratch/user/user NetID
cd $SCRATCH
ls $HOME
```

The Search Path

- The shell uses the PATH environment variable to locate commands typed at the command line
- The value of PATH is a colon separated list of full directory names.
- The PATH is searched from left to right. If the command is not found in any of the listed directories, the shell returns an error message
- If multiple commands with the same name exist in more than one location, the first instance found according to the PATH variable will be executed.

echo \$PATH

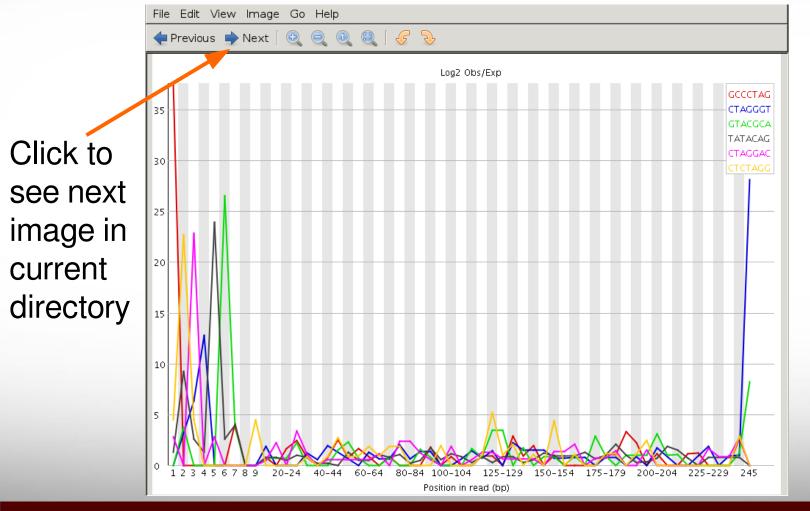
```
PATH=/opt/TurboVNC/bin:/software/tamusc/local/bin:
/software/lsf/9.1/linux2.6-glibc2.3-x86_64/etc:
/software/lsf/9.1/linux2.6-glibc2.3-x86_64/bin:
/usr/local/bin:/bin:/usr/bin:/usr/local/sbin:/usr/sbin:
/sbin:/usr/lpp/mmfs/bin:/opt/ibutils/bin:/home/user_NetID/bin
```

add a directory to the PATH for the current UNIX session

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

Viewing image files with Eye of Gnome image viewer

eog kmer_profiles.png



The 'find' Command

find [target dir] [expression]

```
find ./ -name "*.txt"

find $SCRATCH -mtime -2 -type f

find $SCRATCH -mtime +5

find /tmp -user user_NetID
```

Anything in ./ ending in .txt

Files Modified within last 2 days

Modified more than 5 days ago

Owned by user_NetID

. is the same as ./ which means current directory \$SCRATCH is your /scratch/user/user_NetID directory

Command Aliases

Set a shortcut command or alias for the grep command

```
alias grep='grep --color=auto'
```

Try the new alias

```
grep chrX md5sum.txt
```

- To save alias for each login session, add the alias command to your ~/.bashrc file
 - After editing the ~/.bashrc file,
 you will need to run the source
 command for the current session

```
source ~/.bashrc
```

The 'tar' Command

```
tar [options] [tar file] [file or dir name]
```

- Used to "package" multiple files (along with directories if any) into one file suffixed with a .tar suffix by convention.
- Commonly used options
 - x extract files from a tar
 - c create a new tar
 - t list the contents of a tar
 - v verbosely list files processed
 - f use the specified tar file
 - **z** the tar file is compressed

The 'tar' Command - examples

cd

go to your home directory

Package the temp directory into a file called my_hg19.tar

Package the current directory into a compressed file

```
tar -cvzf my_hg19.tar.gz temp
```

Show the contents of the compressed tar file

```
tar -tzf my_hg19.tar.gz
```

Change the name of your original temp directory

```
mv temp temp_old
```

Extract all contents from the compressed tar file

```
tar -xvzf my_hg19.tgz
```

The 'tar' Command

- · Be careful when extracting files (overwriting old files).
- Where files are extracted depends on how they were packaged.
- Always a good idea to check Table of Contents (-t option) before extraction.

Redirection Operators

- redirects input (use this with bsub on Ada)
- > redirects output
- >> appends output
- input from here document
- 2> redirects error
- &> redirects output and error
- >& redirects output and error
- 2>&1 redirects error to where output is going
- 1>&2 redirects output to where error is going

References

Here are some slides from TACC and LSU on the similar subject.

- Linux/Unix Basics for HPC: October 9, 2014 (with video) [TACC]
 https://portal.tacc.utexas.edu/-/linux-unix-basics-for-hpc
- Express Linux Tutorial: Learn Basic Commands in an Hour [TACC]
 https://portal.tacc.utexas.edu/c/document_library/get_file?uuid=ed6c
 16e9-bcbc-4b70-9311-5273b09508b8&groupId=13601

exit

exit the terminal session # can also use Ctrl+d to detach session

Additional Slides

Using SSH - Putty (on Windows)

https://hprc.tamu.edu/wiki/HPRC:Access:Windows#Using_PuTTY

