### **Linux and Command-Line Interface**

Understand basic jargon (shell, path, file permissions, command line) earn common Linux commands Tips on making command-line easier File permissions **Text editors** SSH to connect to cluster

**Eric J. Walter** Director of Research Computing February 4th, 2025

## **Getting Help**

Departments & Offices / ... / Using / Prerequisites

#### **RC/HPC** website

#### USING HPC

Prerequisites

Logging in to HPC systems

**Environment modules** 

Files & Filesystems

Running HPC jobs with SLURM

Compiling & MPI software

Tutorials

Software

Tunneling HTTP for Jupyter



### **HPC Prerequisites**

William & Mary's HPC clusters run on a mixture of **Red Hat Enterprise Linux** and its derivative **CentOS**, so you will need basic **Unix/Linux** knowledge to use the university's HPC systems. If you are unfamiliar with the Unix/Linux command-line, please avail yourself of one or more of the following resources:

- Unix-the Bare Minimum
- UNIX / Linux Tutorial for Beginners
- Writing tcsh shell scripts
- The Linux command line for beginners (Ubuntu focused)

W&M users also have access to many relevant technical e-books through Swem Library, including Unix Power Tools (also available in print), Learning the Unix Operating System (also available in print), Using csh & tcsh, Linux Pocket Guide: Essential Commands, and Unix in a Nutshell.

#### **Text editors**

As part of your command-line proficiency, you will want to be familiar with some kind of "plain text" editor. Every W&M HPC login server has at least vim, nano, and emacs, of which nano is the easiest for a beginner (but ultimately least powerful). Alternatively, some users prefer to do their editing on their desktop or laptop computers (with the text editor or IDE of their choice), and then use a file transfer utility such as FileZilla, PuTTY, WinSCP, Fetch, rsync, or sftp to copy files to and from the clusters.

HPC webpage: HPC ticket system https://www.wm.edu/it/rc mail: hpc-help@wm.edu

# **Research Computing Staff**



Eric J. Walter Director



Matt Kennedy Network, Filesystem and Data Specialist



Yang Li Research Computing Assistant



Xiao Liang Assistant Director



**Daanish Fiaz** Systems Engineer



**Jay Kanukurthy** Applications Analyst



Malcolm Slaughter Research Computing Specialist



Chris Carpenter Infrastructure Services Architect (VIMS)

### We are located on 1st floor of ISC3.

## The Linux Command Line Interface (CLI)

**Windows, MacOS** have some command-line features - "dos prompt", "run", "powershell" for Windows or "terminal" for MacOS (BSD shell)

Most of you are probably familiar with Graphical User Interfaces (GUI).

Linux especially for HPC is largely command-line. Some GUI interfaces, **but** command-line interface (CLI) can be and often is superior.

- **command Line** Text based interface that lets you interact with computer
- **shell** program that presents the command-line interface
- terminal program that runs a shell
- *prompt* beginning of command line which prompts you for action

Shells come in different flavors (tcsh, bash, zsh, ksh, fish, etc. ) On W&M/VIMS clusters, tcsh is default shell, users can request bash Everything today will be shell agnostic

#### What shell am I running?:



prompt (line number increments with each command)

Other Linux Tutorials - <a href="https://www.wm.edu/offices/it/services/researchcomputing/using/prereqs/index.php">https://www.wm.edu/offices/it/services/researchcomputing/using/prereqs/index.php</a>

## Files/folders/paths

### Windows



### Mac

		🚞 Cache	S	
< >		* · (1) 🖸		Q Search
Favorites  All My Files  Icloud Drive  AirDrop  AirDrop  Applications  Desktop  Documents  Downloads  Devices  Remote Disc  Shared  OSXDaily.com  Writing  Yellow	<ul> <li>Aseventsd</li> <li>PKInstallSandboxManager</li> <li>Spotlight-V100</li> <li>Trashes</li> <li>Vol</li> <li>Applications</li> <li>bin</li> <li>cores</li> <li>etc</li> <li>home</li> <li>installer.failurerequests</li> <li>Library</li> <li>net</li> <li>Network</li> <li>private</li> <li>sbin</li> <li>System</li> <li>tmp</li> <li>Users</li> <li>usr</li> <li>Var</li> <li>Volumes</li> </ul>	<ul> <li>Jocalized</li> <li>Application Support</li> <li>Audio</li> <li>Caches</li> <li>ColorPickers</li> <li>ColorSync</li> <li>Components</li> <li>Cortextual Menu Items</li> <li>CorteMedial0</li> <li>Desktop Pictures</li> <li>Dictionaries</li> <li>DictoryServices</li> <li>Documentation</li> <li>Extensions</li> <li>Filesystems</li> <li>Fonts</li> <li>Frameworks</li> <li>Graphics</li> <li>Image Capture</li> <li>Internet Plug-Ins</li> </ul>	<ul> <li>.DS_Store</li> <li>com.apple.ATimeZone.plist</li> <li>com.apple.CioComponents</li> <li>com.apple.Ce.Components</li> <li>com.apple.dep.admin.png</li> <li>com.apple.Diorks.New.plist</li> <li>com.apple.DiDatabase.501</li> <li>com.apple.ImDatabase.501</li> <li>com.apple.Spotlight</li> </ul>	com.apple.desktop.ad min.png PNG imace - 1.2 MB Created 3/20/15, 2:33 PM Modified 3/20/15, 2:33 PM Last opened 3/20/15, 2:33 PM Dimensions - Add Tags
		1 of 11 selected, 151.52 0	B available	





*mkdir* – *make directory* **cd** – change directory *rmdir* – *remove directory* rm – remove file mv – move / rename file **cp** – copy file ls – list contents of current directory **cat** – dump file to screen history – CLI history (!) **clear** – clear the screen \* – wildcard symbol

#### Special chars for files and directories:

- current directory
- ... up one directory
- ~ home directory
- *previous directory*

**cd** – by itself means cd to home

### **Common Linux CLI Commands**

31 [bora] pwd	print working directory	45 [bora] cp dirlist newdir	copy file "dirlist" into newdir
<pre>/sciclone/home/ewalter/LinuxPre</pre>	S	46 [bora] ls	list contents (nothing changed)
32 [bora] mkdir newdir1	make directory "newdir1"	dirlist newdir	
33 [bora] mkdir newdir2	make directory "newdir2"	47 [bora] ls newdir	list contents of "newdir"
34 [bora] ls	list contents of current dir	dirlist	
newdir1 newdir2		48 [bora] cp dirlist dirlist2	make copy of dirlist named dirlist2
35 [bora] cd newdir1	go into "newdir1"	49 [bora] ls	list
36 [bora] 1s	list current content (it is empty)	dirlist dirlist2 newdir	
37 [bora] cd	go up one directory	51 [bora] cp dir* newdir	cp all files starting with dir to "newdir"
38 [bora] ls	list current directory	52 [bora] cd newdir	go into newdir
newdir1 newdir2		53 [bora] ls	list
39 [bora] ls > dirlist	send stdout of Is to file "dirlist"	dirlist dirlist2	
40 [bora] cat dirlist	dump "dirlist" to screen	54 [bora] cd	go up one directory
dirlist		55 [bora] cd ~	cd to home directory
newdir1		56 [bora] pwd	print current path
newdir2		/sciclone/home/ewalter	
41 [bora] rmdir newdir2	remove newdir2	57 [bora] cd ~ewalter	cd to home directory (another way)
42 [bora] mv newdir1 newdir	rename newdir1 to "newdir"	58 [bora] pwd	print current path
43 [bora] history	list command history	/sciclone/home/ewalter	
31 20:09 pwd		59[bora] cd ~ewalter/LinuxPres	go to LinuxPres (in my home directory)
32 20:09 mkdir newdir1		60 [bora] pwd	print current path
33 20:09 mkdir newdir2		/sciclone/home/ewalter/LinuxPre	S
35 20:09 cd newdir1		61 [bora] cd	go to home directory (yet another way)
37 20:09 cd		62 [bora] pwd	print current path
38 20:09 ls		/sciclone/home/ewalter	
39 20:10 ls > dirlist		63 [bora] cd -	go to previous directory
40 20:10 cat dirlist		64 [bora] pwd	print current path
41 20:10 rmdir newdir2		/sciclone/home/ewalter/LinuxPre	S
42 20:10 mv newdir1 newdir		65 [bora] cd ~	go home
43 20:10 history		66 [bora] cd /sciclone/home/ewa	lter/LinuxPres absolute path
44 [bora] !38		67 [bora] cd ~	go home
ls	repeat command #38	68 [bora] cd LinuxPres	relative path
dirlist newdir	! - reports what command was		

## Paths, ENV variables, symbolic links

### **PATH** – environmental variable ; list of directories which are searched for executable

#### 22 [vortex] echo \$PATH

In -s <PATH> <TARGET>

/sciclone/home10/ewalter/bin:/usr/local/intel-2018/compilers\_and\_libraries\_2018/linux/mpi/intel64/bin:/usr/local/inte
l-2018/compilers\_and\_libraries\_2018.5.274/linux/bin/intel64:/usr/local/torque-6.1.1.1/bin:/usr/local/torque-6.1.1.1/s
bin:/usr/local/maui-r156-GRes/bin:/usr/local/Modules/3.2.10/bin:/usr/local/torque-6.1.1.1/bin:/usr/local/torque-6.1.1
.1/sbin:/usr/lib64/qt-3.3/bin:/usr/lib64/ccache:/usr/local/bin:/bin:/usr/local/sbin:/usr/local/sbin:/usr/local/sbin:/usr/local/bin:/usr/local/sbin:/usr

### Current directory (.) is usually not in path – (must type ./<executable>)

#### Symbolic link – allows an alias for another file/directory

<pre>lrwxrwxrwx 1 ewalter hpcf 24 Apr 9 2012 data10 -&gt; /sciclone/data10/ewalter lrwxrwxrwx 1 ewalter hpcf 18 Apr 9 2012 lscr -&gt; /local/scr/ewalter .</pre>	23 [vortex] ls -1			
<pre>lrwxrwxrwx 1 ewalter hpcf 18 Apr 9 2012 lscr -&gt; /local/scr/ewalter .</pre>	lrwxrwxrwx 1 ewalter hpcf	24 Apr 9	2012 data10 -> /sciclone/data10/ewalter	
	lrwxrwxrwx 1 ewalter hpcf	18 Apr 9	2012 lscr -> /local/scr/ewalter	

If you are missing symlinks in your home folder: **restorewmLinks** 

# Switches / hidden files

#### Many Linux commands have options called switches

ls -l ls -ltr or ls -l -t -r rm -r testdir list with "long" option "long" and sort by reverse modification time remove "recursively" **CAREFUL!** 

hidden files *ls -l* vs. *ls –la*  files/folder that being with '.' "dot" files

long vs. short switches *ls -a* vs. *ls --all* 

#### Presence of trailing slash indicates directory

**Note:** directories can be referred to as "**<directory>**" or "**<directory>/**". The presence of the trailing slash (/) can change some commands behavior. e.g.

Consider you want to my the file "newfile" into the directory "newdir" but you forget to make the directory "newdir" ...

1 [bora] mv newfile newdir

renames newfile to newdir

2 [bora] mv newfile newdir/ mv: failed to access 'newdir/': Not a directory complains

print working directory 90 [bora] pwd /sciclone/home/ewalter/LinuxPres 91 [bora] ls -1 list with "-l" switch (*long*) total 8 -rw-----. 1 ewalter hpcf 24 Sep 10 20:50 dirlist -rw-----. 1 ewalter hpcf 24 Sep 10 20:11 dirlist2 drwx-----. 2 ewalter hpcf 10 Sep 10 20:30 newdir 92 [bora] 1s -ltr list with long and reverse by modification time total 8 -rw-----. 1 ewalter hpcf 24 Sep 10 20:11 dirlist2 drwx-----. 2 ewalter hpcf 10 Sep 10 20:30 newdir -rw-----. 1 ewalter hpcf 24 Sep 10 20:50 dirlist 93 [bora] mkdir .hidden make a "hidden" directory 94 [bora] ls -1 list –l total 8 -rw-----. 1 ewalter hpcf 24 Sep 10 20:50 dirlist -rw-----. 1 ewalter hpcf 24 Sep 10 20:11 dirlist2 drwx-----. 2 ewalter hpcf 10 Sep 10 20:30 newdir 95 [bora] ls -la list with -l and -a (for all) total 56 drwx-----. 4 ewalter hpcf 86 Sep 10 20:51 . drwxr-xr--. 173 ewalter hpcf 86016 Sep 10 20:08 ... -rw-----. 1 ewalter hpcf 24 Sep 10 20:50 dirlist -rw-----. 1 ewalter hpcf 24 Sep 10 20:11 dirlist2 drwx-----. 2 ewalter hpcf 10 Sep 10 20:51 .hidden the hidden directory drwx-----. 2 ewalter hpcf 10 Sep 10 20:30 newdir 96 [bora] ls -a Short list all files with –a . .. dirlist dirlist2 .hidden newdir Short list with –all 97 [bora] ls --all . .. dirlist dirlist2 .hidden newdir 98 [bora] 99 [bora] rmdir newdir Try removing non-empty dir rmdir: failed to remove 'newdir': Directory not empty remove – r recursively 100 [bora] rm -r newdir 101 [bora] ls dirlist dirlist2

# du, df, find

*df* – get filesystem usage (*df* –*h*) *du* – get current directory disk usage

find – find a file

**df** and **du** are important in HPC since you share file-systems with other users.

**du** lets you identify large files/folders **df** tells you how full that filesystem is

find . -type d -name <directory name>
Will search for directory

28 [bora] df -h Filesystem	Size	Used	Avail	Use%	Mounted on	df with —h switch ("human readable")
192.168.56.208@o2ib,192.168.56.209@o2ib:/pscr po00-ib:/sciclone/scr10 cm00:/sciclone/home lu00-ib:/sciclone/data10 or00-i8:/sciclone/scr20	273T 219T 16T 360T 73T	102T 38T 12T 334T 25T	172T 181T 3.9T 27T 48T	38% 18% 76% 93% 35%	/sciclone/ps /sciclone/sc /sciclone/hc /sciclone/da /sciclone/sc	scr cr10 ome ata10 cr20
<pre> 28 [bora] pwd /sciclone/home/ewalter/examples 29 [bora] du -hs . 22G total 30 [bora] du -hs * 4.0K CODE_OF_CONDUCT.md 4.0K CODEOWNERS 4.0K CONTRIBUTING.md 436K cpp</pre>					pwd -hs "hun example -hs * us directory	nan-readable" + "summarize" s is 22 GB sage of each file and folder in this /
31 [bora] cd 32 [bora] findname CODEOWNERS examples/CODEOWNERS					cd up on find file r this direc	e level named "CODEOW NERS" in or below ctory

## Tab completion / up arrow / man

Some really helpful commands...

#### tab completion

ls file<tab>

This will complete the word "file" with whatever files/folders in your current directory match this name.

#### up arrow

Hitting the up-arrow key will cycle back through your current history

**man pages** exist for almost all Linux commands *man ls* 

25 [bora] ls data1 data2 runscript	
26 [bora] ls d <tab> -&gt; ls data data1 data2</tab>	
data2	
29 [bora] Is ru <tab> -&gt; Is runscript runscript</tab>	
30 [bora] <up arrow=""> -&gt; ls runscript</up>	
30 [bora] <up arrow=""> -&gt; 15 data2 30 [bora] <up arrow=""> -&gt; 1s</up></up>	
31 [bora] man ls	
LS(1) User Commands LS (1) NAME	
ls - list directory contents SYNOPSIS	
ls [OPTION] [FILE]	
List information about the FILEs (the current directory by default). Sort alphabetically if none of -cftuvSUX norsort is specified.	entries
Mandatory arguments to long options are mandatory for short options too.	
-a,all do not ignore entries starting with .	
-A,almost-all do not list implied . and	
author with -1, print the author of each file	
•	

# Grep / tar / gzip, bzip2

#### tar and gzip/bzip2 files:

*tar* – tape archive *gzip* – GNU zip *bzip2* – Another zip program

*tar* – combine files into single file collection -- **does not compress** 

Often combined with *gzip* or *bzip2* to compress a tarfile (tarball)

gzip - compresses a file -> file.gz bzip2 - also compresses a file > file.bz2

There other types/suffixes (.xz) See: <u>https://www.geeksforgeeks.org/tar-</u> <u>command-linux-examples/</u> For more in depth discussion

37 [bora] grep pytorch README.md ![Run Examples](https://github.com/pytorch/examples/workflows/Run%20Examples/badge.svg) https://pytorch.org/examples/ `pytorch/examples` is a repository showcasing examples of using 38 [bora] grep pytorch README.md |grep ! ![Run Examples](https://github.com/pytorch/examples/workflows/Run%20Examples/badge.svg) 39 [bora] 115 [bora] pwd /sciclone/home/ewalter/LinuxPres 116 [bora] ls FILES 117 [bora] ls FILES file1 file2 file3 otherfiles 118 [bora] tar czvf FILES.tgz FILES/ FILES/ FILES/otherfiles/ FILES/otherfiles/file4 FILES/otherfiles/file5 FILES/otherfiles/file6 FILES/file1 FILES/file2 FILES/file3 119 [bora] ls FILES FILES.tgz 120 [bora] tar tzvf FILES.tgz drwx----- ewalter/hpcf 0 2023-09-11 17:50 FILES/ drwx----- ewalter/hpcf 0 2023-09-11 17:49 FILES/otherfiles/ -rw----- ewalter/hpcf 0 2023-09-11 17:49 FILES/otherfiles/file4 -rw----- ewalter/hpcf 0 2023-09-11 17:49 FILES/otherfiles/file5 -rw----- ewalter/hpcf 0 2023-09-11 17:49 FILES/otherfiles/file6 -rw----- ewalter/hpcf 0 2023-09-11 17:49 FILES/file1 -rw----- ewalter/hpcf 0 2023-09-11 17:49 FILES/file2 -rw----- ewalter/hpcf 0 2023-09-11 17:49 FILES/file3

### **File/Folder Permissions**



File/folder permissions important for sharing files with others within the HPC clusters.

e.g. Want to allow everyone to copy *file1* out of my home directory:

77 [bora] ls -l file1
-rw 1 ewalter hpcf 6 Jun 7 18:40 file1
78 [bora] ls -ld /sciclone/home/ewalter
drwx 173 ewalter hpcf 86016 Sep 12 12:17 /sciclone/home/ewalter
79 [bora] chmod go+rx /sciclone/home/ewalter
80 [bora] ls -ld /sciclone/home/ewalter
drwxr-xr-x. 173 ewalter hpcf 86016 Sep 12 12:17 /sciclone/home/ewalter
81 [bora] chmod go+r file1
82 [bora] ls -l file1
-rrr 1 ewalter hpcf 6 Jun 7 18:40 file1

In depth discussion of Linux file permissions:

https://www.redhat.com/en/blog/linux-file-permissions-explained

Permissions discussed more in next presentation (tomorrow)

### **Text Editors**

#### To create / edit files, need to use a **text editor**. All HPC systems have: *vi/vim*, *emacs*, and *nano*

*Nano* is most useful for beginners <u>https://www.howtogeek.com/42980/the-beginners-guide-to-nano-the-linux-command-line-text-editor/</u>



List of commands at bottom of screen: i. e. cntrl-X = exit, cntrl-O = write file

### Also, can set up visual studio code to connect to files on HPC via ssh.

### **SSH to Cluster**

ssh – is the standard app for connecting to a remote computer with Linux.
 Standard software on Linux. Mac also supports ssh via *terminal*.
 Windows users can use *powershell* to do this or use ssh client program (*putty*).

For on W&M/VIMS campus or within W&M/VIMS VPN
ssh to bora - ssh ejwalt@bora.sciclone.wm.edu

From off-campus - need to jump through bastion host
ssh to bora through bastion host - ssh -J ejwalt@bastion.wm.edu ejwalt@bora.sciclone.wm.edu

Can configure your local ssh to jump through bastion host automatically:

#### My off-campus ~/.ssh/config file:

Host bora.sciclone.wm.edu HostName bora.sciclone.wm.edu ProxyJump ejwalt@bastion.wm.edu User ewalter

### Is my username the same on my local machine?

If it is different use: ssh <username>@<host>.<domain>

**Do I need graphics?** If yes, must log in with –Y

#### See website for more in depth help:

https://www.wm.edu/offices/it/services/researchcomputing/using/connecting/ https://www.wm.edu/offices/it/services/researchcomputing/using/xfers/

- connecting/logging in to HPC

- transferring files to/from HPC