# HIGH PERFORMANCE RESEARCH COMPUTING

Intermediate Linux

10:00 am Sept. 27, 2022 Short Course



High Performance Research Computing



### Overview

- Text Processing
- Text Processing Practice
- Break
- Bash Scripting
- Bash Scripting Practice
- bc
- Break
- Setting Up an Environment



## **Practice Files**

Login to FASTER now

- Change to your SCRATCH directory
  - o cd \$SCRATCH

- Copy the practice files
  - cp -r /scratch/training/Int\_Linux Int\_Linux



# **Text Processing**

Students will be able to use vi to view, edit and save text files. Students will also be able to understand common uses of stream editors, sed, awk, and grep.



## vi editor

- vi filename # opens (creates) a file using vi
- vi -R filename opens a file using vi in read-only mode
- view filename same as vi-R filename

#### Two modes

- insert mode for typing in text all keystrokes are interpreted as text
  - i one of the commands that initiates insert mode
- command mode
   for navigating the file and editing
   all keystrokes are interpreted as commands
   Esc returns the user to command mode

## vi editor - Practice

Create a file (choose your own filename) using:

• vi filename



## vi editor

"filename"

starts in command mode

press Esc on the keyboard to return to command line mode

Typing :set showmode while in command mode will display in the lower right hand corner what mode you are in

#### To exit a file or save

- **zz** or :wq or :x save the file and exit
- :w filename save the file with the name filename
- :w! force save
- :q or :q! quit without saving
- :q quits a file when there have been no changes
- :q! quits the file regardless of changes

Try writing something, then close the file you created!

#### Open ex01.txt in vi to practice these commands

### Moving around in the file

- h, l (or space), j and k left, right, down and up
- **G** move to end of file
- nG go to line n
- **^f** (**^** = Ctrl-key) Scroll down a full screen
- **^b** scroll up a full screen
- 0 (zero) Move to start of current line
- w move forward one word
- b move back one word
- e move to the end of the word

### Commands that take you into insert mode

- i insert text to the left of the cursor
- I insert text at the beginning of the line
- a insert text to the right of the cursor
- A insert text at the end of the line
- o open a line below the cursor
- o open a line above the cursor
- R overwrite text to the right of the cursor
- cw change a word with new text the cursor must be at the beginning of the word

## vi commands - Practice

- Open a new text file with vi.
- Change vi to insert mode and type "Hello World".
- Then save and exit the file.
- Type Is, do you see the file you created?
- Type more filename, if saved you should see "Hello World"



Editor commands that keep you in command mode

- x delete a single character at the cursor
- dd delete the entire current a line
- ndd delete n lines
- dw delete a word
- dG delete to the end of the file
- D delete to the end of the line
- replace current character with a (a = character, number, etc.)
- u undo last command (only 1 undo on most unix machines. Most new versions of vi (vim) have multiple undo and redo (Ctrl-r) capability)
- nyy yank n (n is a number) lines to memory
- p (lowercase p) put the yanked lines below the cursor
- P (uppercase P) put the yanked lines above the cursor



#### Miscellaneous commands

- Iname search forward for name
- o ?name search backward for name
- o :1,\$ s/pattern1/pattern2/g
  - from line 1 to the bottom find and substitute pattern1 for pattern2
  - you could also use :% s/pattern1/pattern2/g
    - % and 1,\$ mean the entire file
    - the g means that all occurrences of pattern1 will be substituted in a line and not just the first one
- :e filename exits to the file filename
- o ma marks that line and stores the position in the variable a
- o : 'a, . y x yanks the lines between the mark a and where the cursor is (.) and stores it in the variable x
- o :pu x puts the lines stored in x into the file where the cursor is
- o :r filename read file named filename and insert after current line
- :set all lists all of the settings
- :set number displays line numbers



## vi commands - Practice

- Navigate to Int\_Linux in your scratch dir and open the file ex01.txt
- type wc -I to see how many lines are in the file.
- Search forward for the string "Atoms" in the file. What line is it on?
- Use the dd command to delete this line.
- Type **G** to jump to the end of the file.
- Type gg to jump to the beginning of the file.
- Then quit without saving.

## GNU sed - Stream editor

A stream editor is used to perform basic transformations on text read from a file or a pipe.

- man sed
  - man displays user manual information about commands
- Useful one-line scripts for sed: <a href="http://sed.sourceforge.net/sed1line.txt">http://sed.sourceforge.net/sed1line.txt</a>
- Online manual: <a href="https://www.gnu.org/software/sed/manual/">https://www.gnu.org/software/sed/manual/</a>
- Common uses
  - o sed -n '4,6p' filename
    - print out line 4 to line 6 (without –n, line 4 to 6 will be printed twice)
  - o **sed** '2,4**d'** filename
    - delete line 2 to line 4
  - o sed '3,\$d' filename
    - delete line 3 to the last line of the file

## GNU sed - Stream editor

- s substitute
  - o sed 's/pattern1/pattern2/g' filename
    - find pattern1 and replace it with pattern2, output is set to stdout
  - o sed 's/pattern1/pattern2/g' filename > filename2
    - output is set to filename2
  - o **sed** -i 's/pattern1/pattern2/g' filename
    - modifies the file in-place (changes the original file)
  - o sed 's/^/pattern1/' filename
    - insert pattern1 at the beginning of each line of a file
  - o sed 's/\$/pattern1/' filename
    - insert pattern1 at the end of each line of a file

### sed - Practice

- In this practice we will use the file ex02.txt.
- Make the following changes to the text file using sed commands.
- cp ex02.txt tmp.txt create a copy of the file to work on.
- Replace all instances of "vegetables" with "cheese" even if it appears more than once in a line.
- Delete the 1st line of the file.
- Delete the now 2nd line of the file.
- Delete the now fourth line of the file.
- Print lines 1 to 4 and save to a file output.txt.

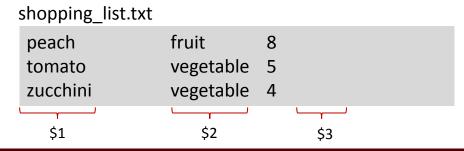


## **GNU Awk**

awk is used to search files for lines (or other units of text) that contain certain patterns and then do something (print, manipulate, etc).

```
awk options '/search pattern/ {action}' input-file > output-file
```

- Delimiters (Field Separator, FS)
  - Default is white space
- Search patterns
  - awk '/pattern/' filename
- Variables
  - fields are stored in variables based on the FS
  - \$0 the entire line
  - \$1 1st field
  - \$2 2nd field



### **GNU Awk**

- Variables
  - NR number of records
  - NF Number of Fields in a record
  - RS Specifies the record separator

- FS Specifies the field separator
- OFS Specifies the Output field separator
- ORS Specifies the Output record separator

- Print statement
  - awk '/pattern/ {print \$0}' filename
  - awk '/pattern/ {print \$1 "," \$2}' filename>outputfilename.txt
- printf statement for more control over the print format
  - https://www.gnu.org/software/gawk/manual/html\_node/Printf-Examples.html
- Pre-processing/Post-processing
  - BEGIN

```
awk 'BEGIN {print "Shopping List"} { print $1, $2 }' sample.txt
```

END

```
awk 'END { print NR }' sample.txt
```

### GNU AWK - Practice

- Print the 3rd column of the tmp.txt file created during the last practice.
- What does it say?



# Searching File Contents - grep

**grep** search-pattern filename - searches the file filename for the pattern search-pattern and shows the results on the screen (prints the results to standard out).

- o grep Energy run1.out
  - searches the file run1.out for the word Energy
  - grep is case sensitive unless you use the -i flag
- o grep Energy \*.out
  - searches all files in that end in .out
- grep "Total Energy" \*/\*.out
  - You must use quotes when you have blank spaces. This example searches for Total Energy in every file that ends in .out in each directory of the current directory
- grep –R "Total Energy" Project1
  - Searches recursively all files under Project1 for the pattern Total Energy



# Searching File Contents - grep

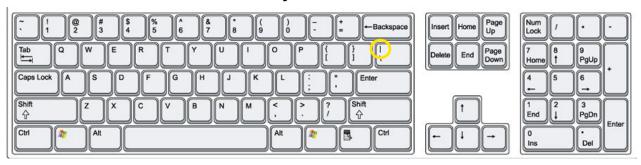
- grep -A N 'search' filename
  - Outputs N lines after each line containing the search term.
- grep -B N 'search' filename
  - Outputs N lines before each line containing the search term.
- grep -v 'search' filename
  - Outputs lines that do not contain the search term.



# Searching File Contents - egrep

### egrep 'pattern1|pattern2|etc' filename

- searches the file filename for all patterns (pattern1, pattern2, etc) and prints the results to the screen.
- The | character is called a pipe and is normally located above the return key on the keyboard.
- egrep 'Energy|Enthalpy' \*.out
  - searches for the word Energy or Enthalpy in every file that ends in .out in the current directory.





grep & egrep Hands on Practice

- Use grep to count the number of lines containing either 'min' or 'max' in the file ex03.txt.
- Using only grep, print only the line after the line containing 'love' in the file ex02.txt

## **10 Minute Break**



# **Bash Scripting**

Learning Objective:

Understand conditions, loops and write bash scripts for simple tasks



## **Basic Shell Scripting**

A shell script is a text file that contains one or more linux commands that can be run as a single batch of commands.

Shell scripts can be used to automate routine tasks.

It is good practice to name shell scripts with: .sh

The shell ignores blank and commented-out lines.
It is a good practice for developers to include info about the script in the header.

To store the output of a command in a variable, use MYVAR=\$ (command)

To run the script

- run with bash script.sh
- add executable permission to the script file (chmod u+x script.sh) and run with ./script.sh



# Basic Constructs for Bash Scripting

Conditionals:

If something is true do something and if it is false, do something else

```
if < some test >
then
   commands
elif < some test >
then
   other commands
else
   commands
fi
```

```
#!/bin/bash
i=1
if [ $i -eq 1 ] ; then
   echo i is equal to 1
  else
   echo i does not equal 1
   echo i equals $i
  fi
```

# **Integer Comparison Operators**

-eq	is equal to	if [ "\$a" -eq "\$b" ]
-ne	is not equal to	if [ "\$a" -ne "\$b" ]
-gt	is greater than	if [ "\$a" -gt "\$b" ]
-ge	is greater than or equal to	if [ "\$a" -ge "\$b" ]
-lt	is less than	if [ "\$a" -lt "\$b" ]
-le	is less than or equal to	if [ "\$a" -le "\$b" ]
<	is less than (within double parentheses)	(("\$a" < "\$b"))
<=	is less than or equal to (within double parentheses)	(("\$a" <= "\$b"))
>	is greater than (within double parentheses)	(("\$a" > "\$b"))
>=	is greater than or equal to (within double parentheses)	(("\$a" >= "\$b"))

# String Comparison Operator

```
True if $a starts with an "z" (pattern matching).
                                                                  [[ $a == z*]]
==
             True if $a is equal to z* (literal matching).
                                                                 [[ $a == "z*" ]]
             File globbing and word splitting take place.
                                                                    [ $a == z* ]
             True if $a is equal to z^* (literal matching).
                                                                 [ "$a" == "z*" ]
                                                                 [ "$a" != "$b" ]
! =
                         is not equal to
                                                            if [[ "$a" < "$b" ]] or</pre>
<
              is less than, in ASCII alphabetical order
                                                               if [ "$a" \< "$b" ]
                                                            if [[ "$a" > "$b" ]] or
>
             is greater than, in ASCII alphabetical order
                                                               if [ "$a" \> "$b" ]
                                                                  if [ -z "$s" ]
                string is null, that is, has zero length
-z
                         string is not null
                                                                  if [ -n "$s" ]
-n
```

## **Basic Constructs for Bash Scripting**

### **Case Constructs**

```
case var in
  case1)
      <commands>
    ;;
  case2)
      <commands>
    ;;
*)
  commands;;
esac
```

\* symbol defines the default case, usually in the final pattern.

```
#!/bin/bash
month='June'
case $month in
  Jan)
    mnum='01'
    ; ;
  Feb)
    mnum='02'
    ; ;
  Dec)
    mnum = '12'
esac
```

## **Practice: Conditionals**

- Create a shell script that checks if the current day on the system belongs to the first, middle or last part of the month.
- If it is within the first 10 days of a month, print (echo) "We are within the first 10 days of the month."
- Otherwise, check if it is less than or equal to 20 and echo "We are within the middle 10 days of the month."
- If none of the previous conditions are met, return "We are within the last few days of the month."
- Hint: To obtain current day of month, use the command date +%d (there is a space before +)

## Bash Scripts with input outside the script

Command line arguments

```
#!/bin/bash
# shell script exercise
my_name=$1
echo "Howdy $my_name"
```

```
[user@host ~]bash my_name.sh
Amy
[user@host ~]Howdy Amy
```

Read input during script execution

```
#!/bin/bash
# Ask the user for emails
read -p "Username: " uservar
read -sp "Password(hidden): " passvar
echo
echo Thankyou $uservar we now have your info
```

```
[user@host ~]bash info.sh
Name: Amy
Password(hidden):
[user@host ~]Thankyou Amy
we now have your info
```

Accept data that has been redirected into the Bash script via STDIN



# **Basic Constructs for Bash Scripting**

```
Loops: Do something over and over until a
specific condition changes and then stop
while [ <some test> ]; do
```

```
for var in <list> ; do
```

<commands>

<commands>

done

done

```
((i++))
done

#!/bin/bash
for file in *.log ; do
head -n1 $file
```

while [ \$i -le 100 ] ; do

echo i equals \$i

#!/bin/bash

done

#

i=1

## Practice: Loops

- Write a simple number-guessing game in a script called guess.sh. When the script is launched, a random number between 1 and 10 is generated and stored in the variable RANDOMNUM. The script then will expect input from the user. If the guess is incorrect, it will continue to ask the user for an input until the user guesses the number correctly. (Hint: to generate a random number between 1 and 10, use the command shuf -i1-10 -n1)
- Change the permissions on files end with .sh to 755 using a for loop

#### bc - Basic Calculator

- bc is a command line calculator which can be useful for quick calculations.
  - Allows for arithmetic operations in bash scripts.
- Addition/subtraction Example:
  - echo "13+3" | bc
- Exponential Example:
  - echo "10^3" | bc
- Assign value of calculation to variable example:
  - o x=`echo "12+5" | bc`
  - o echo \$x
- Variables can be used in calculations:
  - echo "\$x+100" | bc
  - What value do you get?

### bc - Practice

- Create a bash script that defines a variable i as 1.
- Then add a loop that adds (i+2) to i, 12 times.
  - Print i each step of the loop.
- What is the final number?



10 Minute Break



# Customizing the Environment



## Bash Environment Variables

- Environment variables store information that is used across different processes in a Linux system.
- Use all caps for Bash Environment variable.
   A-Z 0-9 \_
- Use lowercase for the variables that you create. a-z 0-9 \_
  - HOME Pathname of current user's home directory
  - **PATH** The search path for commands.
- Use the **echo** command to see the contents of a variable

echo \$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

/usr/lib64/qt-3.3/bin:/sw/local/bin:/usr/local/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/usr/local/sbin:/usr

Add a directory to the PATH for the current Linux session

export PATH=\$PATH:/home/netid/bin

### **Customizing the Environment**

Two important files for customizing your Bash Shell environment

- .bashrc (pronounced dot bashrc)
  - o contains aliases, shell variables, paths, etc.
  - executed (sourced) upon starting a non-login shell.
- .bash\_profile (dot bash\_profile)
  - o also can contain aliases, shell variables, paths, etc
  - normally used for terminal settings
  - o executed (sourced) upon login
  - o if .bash\_profile doesn't exist, the system looks for .profile (dot profile)
- . .bashrc (or source .bashrc)
  - o Executes the commands in the .bashrc file



### .bash profile file contents

```
# Get the aliases and functions
    if [ -f ~/.bashrc ]; then
           . ~/.bashrc
    fi
```

# User specific environment and startup programs PATH=\$PATH:\$HOME/.local/bin:\$HOME/bin

# Personal aliases

alias h="history|more" alias m="more"

export PATH

# User specific functions function cc() { awk -f cc.awk "\$@".log>"\$@".cc; }

following command will be executed: awk -f cc.awk test.log > test.cc

A line that begins with a # is a comment Enable settings in .bashrc

> Syntax to set a global variable: export var\_name=value

Specify PATH for all sessions

Add personal aliases

Syntax to create a function: function name() { command ; }

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If you type **cc test** at the prompt, the

### Practice 4: Alias and \$PATH

- Add a new alias in your .bash\_profile under your home directory named simple that executes the command: echo I succeeded in creating a simple alias
- Activate your new alias
- Type simple at the prompt to use your new alias
- Make a directory named **myapps** in your home directory
- Create a file (*your choice of a name*) in **myapps** with the following content:
  - o echo I succeeded in adding *myapps* to my path
- Change the permissions of filename to allow execution (replace filename with the name that you used
- Run filename by typing filename (you should get an error message)
- Add myapps directory to your PATH with export in your current session
- Run filename by typing: filename



### Solution: Alias and \$PATH

 Add a new alias in your .bash\_profile file named simple that executes the command: echo I succeeded in created a simple alias

### echo 'alias simple="echo I succeeded in creating a simple alias" '>> .bash\_profile

- active your new alias
  - . .bash\_profile
- Type simple at the prompt to use your new alias

### simple

Make a directory named myapps in your home directory

```
cd
mkdir myapps
```

- Create a file (your choice of a name) in myapps with the following content:
  - echo I succeeded in adding myapps to my path

```
cd myapps echo "echo I succeeded in adding my apps to my path" >> filename
```

### Solution: Alias and \$PATH

 Change the permissions of *filename* to allow execution (replace *filename* with the name that you used)

```
chmod u+x filename
```

• Run filename by typing filename (you should get an error message)

```
filename
```

bash: filename: command not found

Add myapps directory to your PATH with export in your current session

```
export PATH=$PATH:/root/myapps/
```

• Run filename by typing: filename

```
filename
```



https://hprc.tamu.edu

HPRC Helpdesk:

help@hprc.tamu.edu

Phone: 979-845-0219

Help us help you. Please include details in your request for support, such as, Cluster (Faster, Grace, Terra, ViDaL), NetID (UserID), Job information (Job id(s), Location of your jobfile, input/output files, Application, Module(s) loaded, Error messages, etc), and Steps you have taken, so we can reproduce the problem.

