

Introduction to Linux (Part 3)

-- Shell Scripting

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Linux Virtual Machine

- Get a temporary account (or use your own CHPC account)
- Virtual Machine FastX portal: <https://linuxclass.chpc.utah.edu:3300>
- Open a XFCE Terminal
 - Adjust Font size: Edit → Preferences → Appearance → Click on Font → adjust Font Size
- Use Bash shell (quick check: echo \$SHELL)
- Copy and Paste issue on Mac

Getting the exercise files

```
cd ~
```

```
mkdir LinuxClass
```

```
cd LinuxClass
```

```
wget https://home.chpc.utah.edu/~u6047586/LinuxScripting2.tar.gz
```

```
tar -xvzf LinuxScripting2.tar.gz
```

```
cd LinuxScripting2
```

What is a shell script?

- A script is a series of shell commands stored in a file
- A script can be executed in several ways:
 - `bash scriptname.sh` (`python xxxx.py` or `Rscript xxxx.r`)
 - `./scriptname.sh` (if the script file executable, `rwX r-X r-X`)
 - `scriptname.sh` (if the script is on your **\$PATH environment variable**)
- commands are separated by:
 - new line
 - semi colon “;”
- Commands executed sequentially until
 - the end of the file has been reached
 - an error happens
 - the “exit” command is executed

Scenarios for scripting

- Using the batch system at CHPC (discussed in the talk on Slurm Basics)
- Automating pre- and post- processing of datasets
- Performing lots of menial, soul draining tasks efficiently and quickly
- Preserve/share operations

Exercise 1: Write a first script

Create a file named **my_ex1.sh** using nano.

First line always contains **'#!'** followed by the language interpreter. ("shebang")

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

```
echo "My first script:"
```

```
echo "My user name is:"
```

```
whoami
```

```
echo "My HOME dir is at"
```

```
echo $HOME
```

```
MSG1="I am in the directory:"
```

```
echo $MSG1
```

```
pwd
```

```
MSG2="Today's date:"
```

```
echo $MSG2
```

```
date
```

```
echo "End of my first script."
```

User-defined Variables



Run the script:

```
bash my_ex1.sh
```

Or, make the script executable first:

```
chmod +x my_ex1.sh
```

Then run your script:

```
./my_ex1.sh
```

Script Arguments

Command line arguments to a script are available in the script as **\$1**, **\$2**, and so on.

For example, if a script is named “myscript.sh” and the script is executed with “**./myscript.sh value1 value2 value3**”:

- the pre-defined internal variable **\$1** has the value “value1”
- the variable **\$2** has the value “value2”
- the variable **\$3** has the value “value3”
- **\$0** contains the name of the script
- **\$#** contains the # arguments
- **\$*** contains all arguments

Try it out

- 1) Create a new script "test_args.sh"
- 2) chmod +x test_args.sh
- 3) ./test_args.sh a b c

```
#!/bin/bash
echo "script name: $0"
echo "how many arguments: $#"
```

echo "list all arguments: \$*"
echo "arg1: \$1"
echo "arg2: \$2"
echo "arg3: \$3"
echo "done"

Re-cap: Different Variables

Environmental Variables:

eg \$HOME, \$PATH \$USER

Internal Variables in Bash Script:

eg \$0, \$1, \$2, \$*, \$#

User-defined Variables:

MY_VAR="this is my first var!"

echo \$MY_VAR

Saving **results** of a command to a user-defined Variable

- The **result** of a command can be put directly into a variable with the **backtick**: `
- The backtick is not the same as a single quote:

Backtick: ` Single quote: ‘

- For example: (no spaces around = sign)

```
VAR=`wc -l $FILENAME`
```

- You can also do this:

```
VAR=$(wc -l $FILENAME)
```

String replacement

Beyond prefix and suffix: <prefix>-\$file; \$file-<suffix>

A neat trick for changing the name of your output file is to use string replacement to mangle the filename.

```
#!/bin/bash
IN="myfile.in"
#changes myfile.in to myfile.out
OUT=${IN/.in/.out}
./my_program $IN > $OUT
```

- In bash, `${VAR/search/replace}` is all that is needed.
- You can use the `sed`, `awk`, or `tr` commands for more powerful manipulations.

Exercise 2.0

Write a script (`my_ex2.sh`) that takes a file name as an argument, searches that file for exclamation points with **grep**, puts all the lines with exclamation marks “!” into a new file named “outfile”, and then counts the number of lines in outfile. Use “histan-qe.out” (output file of a Materials Science software) as your test file.

Don't forget **#!/bin/bash**

Variables - Bash style: **VAR="string"** (no spaces!)

Arguments - **\$1 \$2 \$3 ...**

Grep - **grep 'string' filename**

Counting Lines - **wc -l filename**

Solution to Exercise 2.0

Script my_ex2.sh

```
#!/bin/bash
INPUT=$1
grep "!" $INPUT > outfile
cat outfile | wc -l
```

The output from your script should have been “34”.

Dates and Times

- Date strings are easy to generate in Linux
 - “date” command gives the date,
Fri Sep 8 09:59:02 MDT 2023
but not nicely formatted for filenames
 - “date --help” will give format options (use +)
- `date +"Today is: %D"` “Today is 05/31/18”
- `date +%r` ”10:51:17 AM”
- `date +%Y-%m-%d_%H-%M-%S_%N`
“2014-09-15_17-27-32_864468693”

Exercise 2.1

Modify your previous script so that instead of writing to an output file with a fixed name, the output filename is derived from the input file (e.g., ‘XXXX.out’ becomes ‘XXXX.todays_date’). Don’t forget to copy your script in case you make a mistake!

Command execution to string - **VAR=`command`** (use the backtick) or **VAR=\$(command)**

Bash replacement – **\${VAR/search/replace}**

Dates - **date +%Y-%m-%d_%H-%M-%S_%N** (or pick your own format)

Solution to Exercise 2.1

```
#!/bin/bash
INPUT=$1
DATE=`date +%Y-%m-%d_%H-%M-%S_%N`
OUT=${INPUT/out/$DATE}
grep "!" $INPUT > $OUT
wc -l $OUT
```

Every time you run the script, a new unique output file should have been generated.

Conditionals (If statements)

```
#!/bin/bash
VAR1="name"
VAR2="notname"
if [ "$VAR1" == "$VAR2" ]
then
    echo "VAR1 and VAR2 have the same value."
else
    echo "VAR1 and VAR2 have different values."
fi
if [ -d "$VAR1" ] then
    echo "$VAR1 is a directory!"
else
    echo "$VAR1 is not a directory!"
fi
```

- The operators ==, !=, <, >, &&, || and a few others work.
- The “else” clause is optional.
- You can test variable values and file properties.
- See the manual page with “man test” for all the options.

Conditionals (File properties)

Test	bash
Is a directory	- d
If file exists	- a , - e
Is a regular file (like .txt)	- f
Readable	- r
Writable	- w
Executable	- x
Is owned by user	- O
Is owned by group	- G
Is a symbolic link	- h , - L
If the string given is zero length	- z
If the string is length is non-zero	- n

- The last two flags are useful for determining if an environment variable exists.
- The rwx flags only apply to the user who is running the test.

Loops (for statements)

```
#!/bin/bash
for i in 1 2 3 4 5
do
    echo $i
done
for i in *.in
do
    touch ${i/.in/.out}
done
for i in `cat files`
do
    grep "string" $i >> list
done
```

- Loops can be executed in a script --or-- on the command line.
- All loops respond to the wildcard operators *, ?, [a-z], and {1,2}
- The output of a command can be used as a for loop input.
- There are also while and until loops.

Exercise 2.2

Run the script called ex2.sh. This will generate a directory "ex2" with 100 directories and files with different permissions. Write a script (my_ex22.sh) that examines all the directories and files in "ex2" using conditionals and for loops. For each iteration of the loop:

1. Test if the item is a directory. If it is, delete it.
2. If the file is not a directory, check to see if it is executable.
 - A. If it is, then change the permissions so the file is not executable.
 - B. If the file is not executable, change it so that it is executable and rename it so that it has a ".script" extension.
3. After all the files have been modified, execute all the scripts in the directory.

For loops : **for VAR in *; do ... done**

If statements : **if [condition]; then ... else ... fi** Useful

property flags - **-x** for executable, **-d** for directory

-You can reset the directory by re-running the script ex2.sh

-Make sure that you do not write your script in the ex2 directory, or it will be deleted!

Solution to Exercise 2.2 (my_ex22.sh)

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

```
for i in ex2/*
do
  if [ -d $i ]
  then
    rm -rf $i
  else
    if [ -x $i ]
    then
      chmod -x $i
    else
      chmod +x $i
      mv $i $i.script
    fi
  fi
done
for i in ex2/*.script
do
  ./$i
done
```

Basic Math

```
#!/bin/bash
#initialization
i=1
#increment
i=$(( i++ ))
#addition, subtraction
i=$(( i + 2 - 1 ))
#multiplication, division
i=$(( i * 10 / 3 ))
#modulus
i=$(( i % 10 ))
#not math, echo returns "i+1"
i=i+1
```

- Bash uses `$(())` for arithmetic operations.
- Important! This only works for integer math. If you need more, use Python, R, etc.

Bash “Strict” Mode

- Some bash settings simplify debugging:

```
set -e          #Exit immediately on any command returns errors
set -u          #Error if referencing undefined variable
set -o fail     #Error on any pipe command
```

```
# Example: this code should fail:
```

```
pattern="somestring $some_undefined_variable"
grep $pattern non_existent_file | wc -l
```

- You can do this all at once (put after shebang):

```
set -euo pipefail
```

- See Aaron Maxwell’s blog:

– <http://redsymbol.net/articles/unofficial-bash-strict-mode/>

- Also helpful is “bash -x yoursript.sh” or “set -x”: prints each line before execution

More on scripting techniques

- Create functions

```
my_func() {  
    echo "Today is $1"  
}  
  
my_func "Friday"  
my_func "a big day!"
```

- Single quotes ‘ ’ V.S. Double quotes “ ”

```
MY_VAR=1  
echo "The value is $MY_VAR" #Expand variable into value: The value is 1  
echo 'The value is $MY_VAR' #Preserve literal string: The value is $MY_VAR
```

- Redirect the standard error

```
command # Output (stdout) and Error (stderr) printed on Screen  
command > out.txt # Save Output to a file; Error printed on Screen  
command 2> error.txt # Save Error to a file; Output printed on Screen  
command > out.txt 2>error.txt # Save output and Error to different files  
command &> logs.txt (or command > logs.txt 2>&1) # Save both to same file
```

Thank You

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