Advanced Scientific Programming

Part 1 Linux and Shell

D. S. Hwang

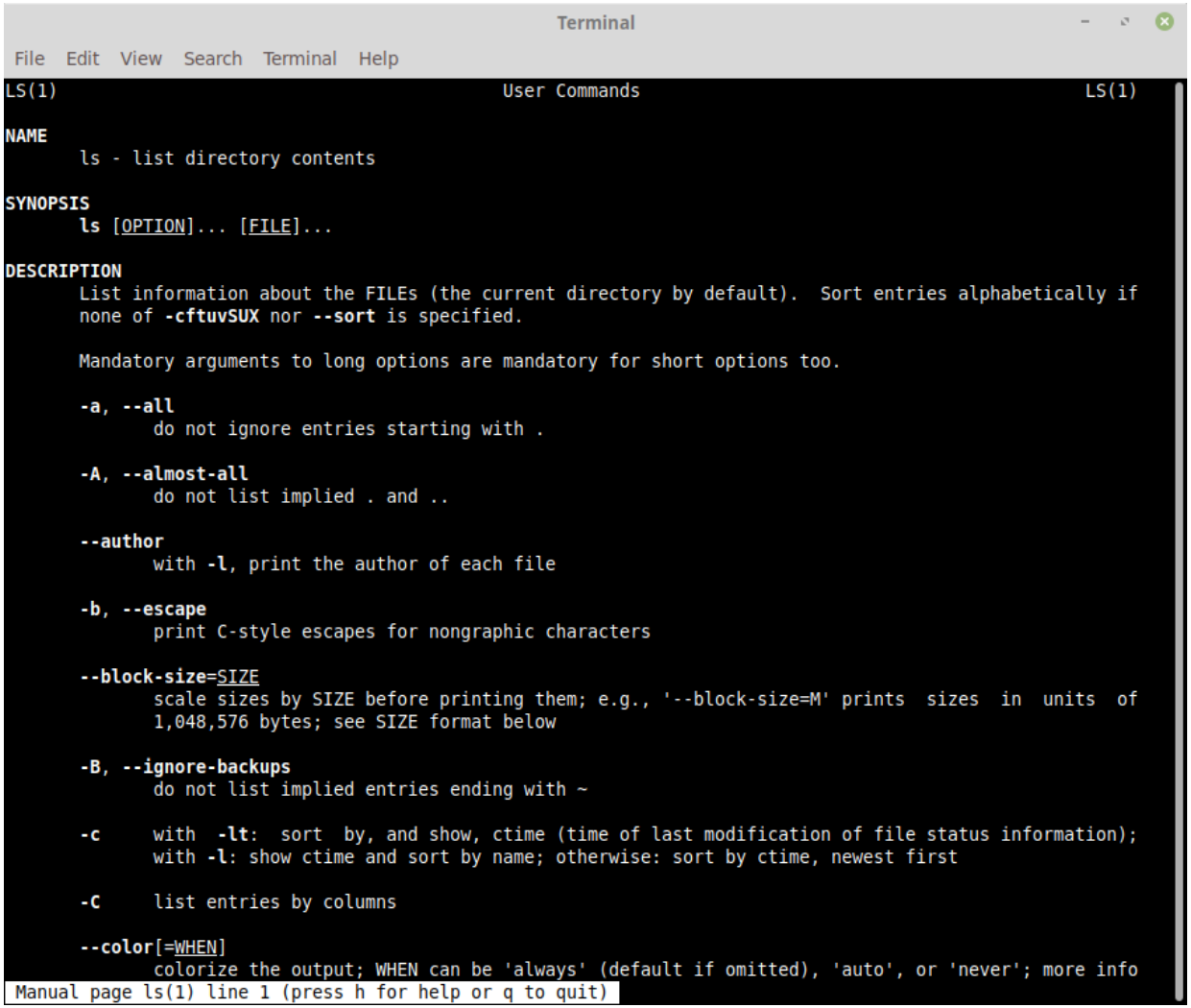
Dankook University

April 23, 2020

The Linux Shell I

- Provides a command line interface(CLI) to the operating system
- Large variety of shells: `bash`, `tcsh`, `csh`, `ksh`, `zsh`
- Let us review commands for `bash`, the default on most systems
- Documentation can be found by typing `man <command>`, e.g. `man bash`

The Linux Shell II



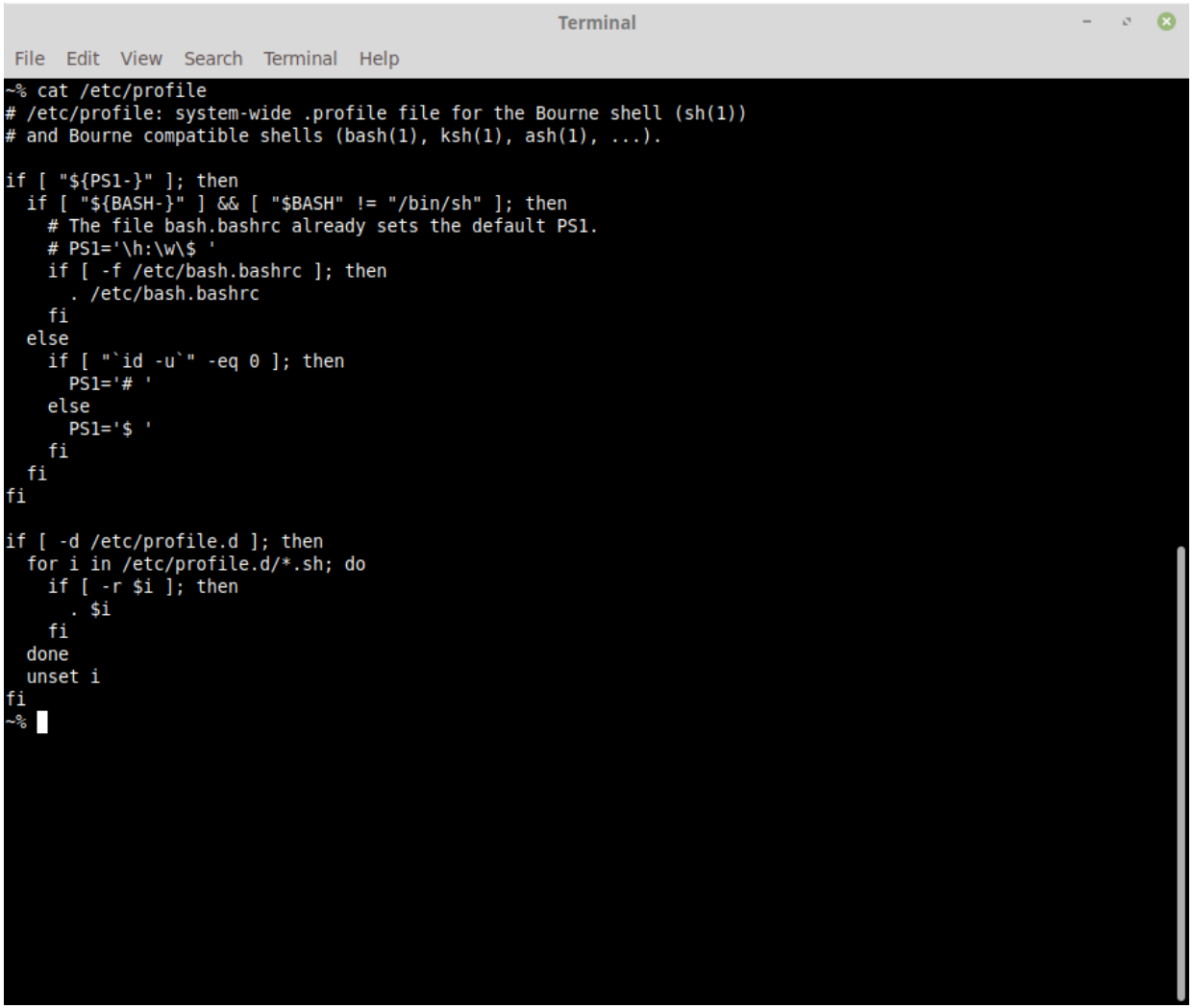
The Linux Shell III

- On login the system executes:
  - System file: `/etc/profile`, `/etc/bashrc`
  - For login shells, run `~/.bashrc`
  - For non-login shells, run `~/.bashrc_profile`
- Bash start-up files
  - `/etc/profile` sets an environment and defines start programs for all users
  - `/etc/bashrc` defines aliases and functions for all users
  - `~/.bash_profile` sets an environment and defines start programs for a user
  - `~/.bashrc` defines aliases and functions for a user
- To avoid complications it's recommended to have your `~/.bashrc_profile` as a symlink to `~/.bashrc`.
- The execution order for start-up files is `/etc/profile`, `~/.bash_profile`, and `~/.bashrc`.

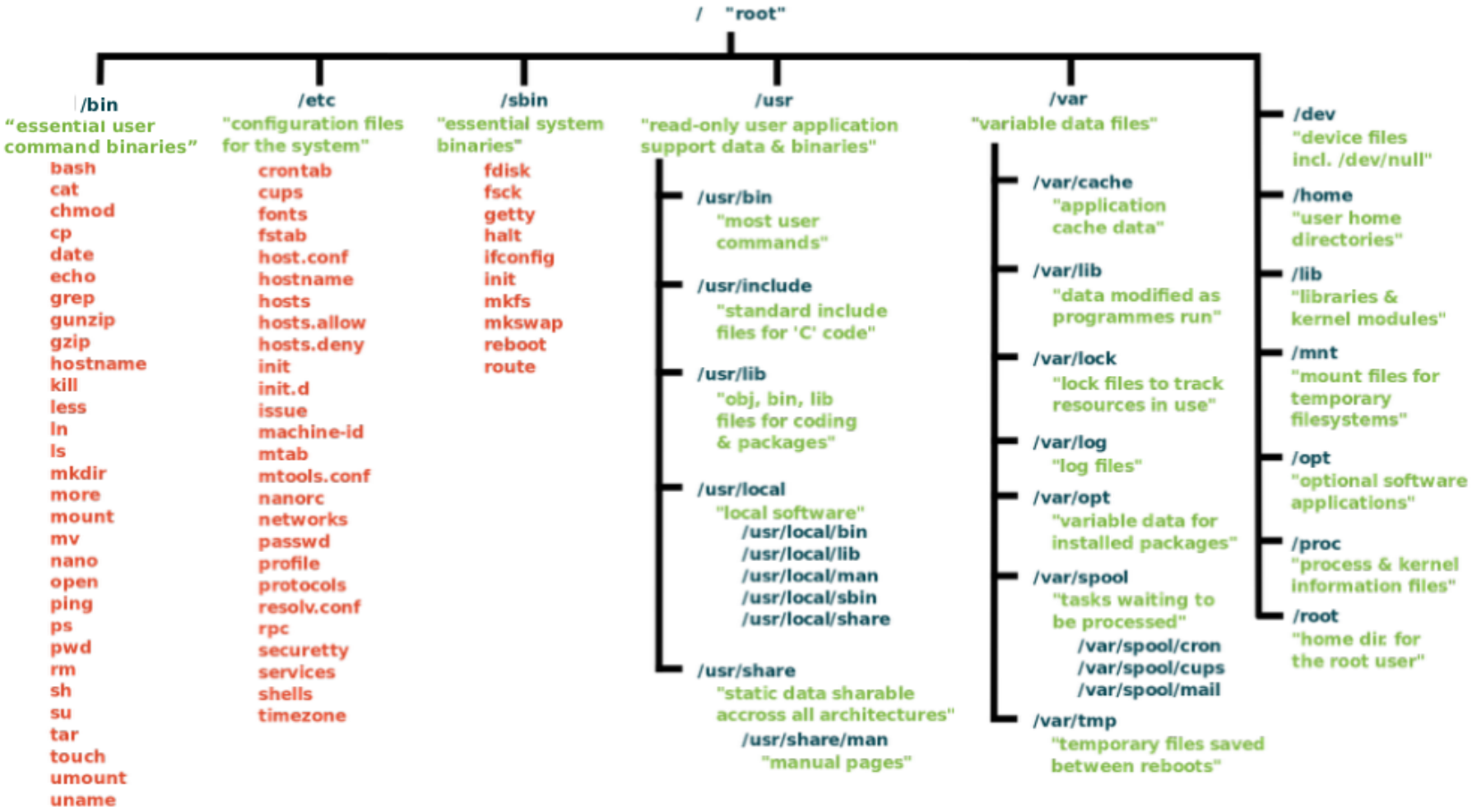
The Linux Shell IV

- The shell checks the first line of every program and if it finds `#!<interpreter>` it uses the the given interpreter to evaluate the file(e.g. `#!/usr/bin/env python`)
- `bash` is a very powerful shell that can be used for input redirection (`<`,`>`, `&`, `...`), job control (fg, bg, jobs), file globbing (*, [0-9], ...).
- Check the `man` page for more!

The Linux Shell V



Standard File System I



Standard File System II

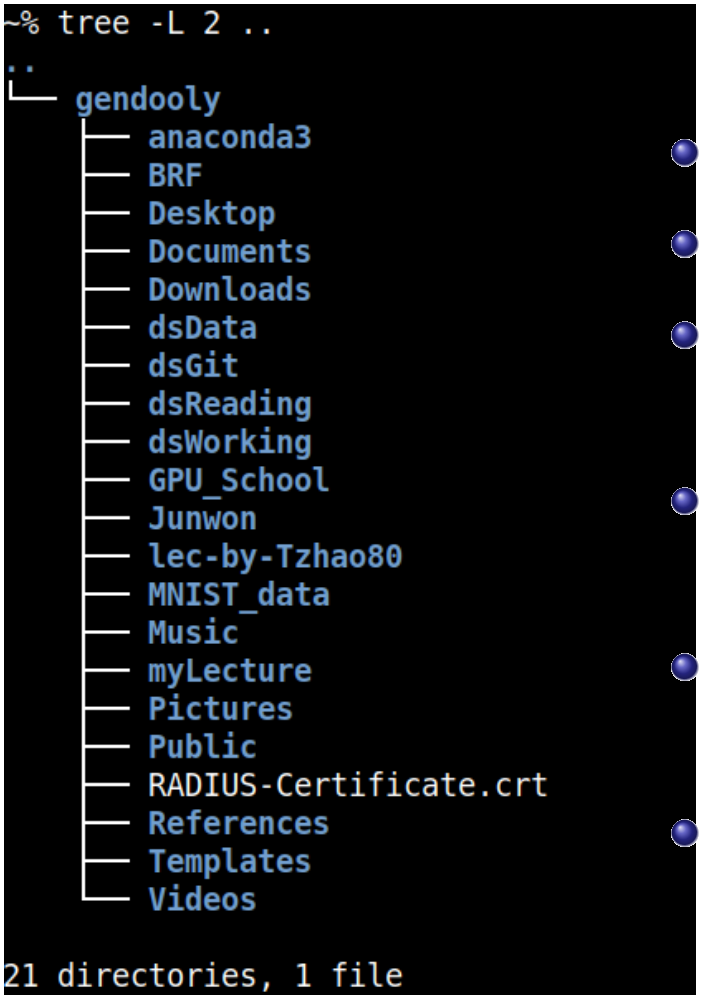
```
~% tree -L 1 /
/
├── bin
├── boot
├── cdrom
├── core
├── dev
├── etc
├── home
├── initrd.img -> boot/initrd.img-4.15.0-91-generic
├── initrd.img.old -> boot/initrd.img-4.15.0-44-generic
├── lib
├── lib64
├── lost+found
├── media
├── mnt
├── opt
├── proc
├── root
├── run
├── sbin
├── srv
├── swapfile
├── sys
├── timeshift
├── tmp
├── usr
├── var
├── vmlinuz -> boot/vmlinuz-4.15.0-91-generic
└── vmlinuz.old -> boot/vmlinuz-4.15.0-44-generic

22 directories, 6 files
```

Standard File System III

- /bin and /usr/bin contain standard Linux commands
- /sbin and /usr/sbin contain system administration commands(`/sbin` stands for "safe" bin)
- /lib and /usr/lib contain standard Linux libraries
- /dev contains device drivers
- /var contains configuration and log files
- /etc contains default configuration files
- /usr/local/bin contains commands not a part of the distribution, added by the administrator on the installed Linux
- /opt contains commercial software
- /tmp stores temporary files

Home Directory I



- gendooly is my home directory.
- Desktop is the directory for the desktop.
- Documents is the default directory for documents.
- Downloads is the recommended directory for downloaded files.
- Public is the folder that is shared on File Sharing.
- Videos is the default directory for music and media files.

Basic Command I

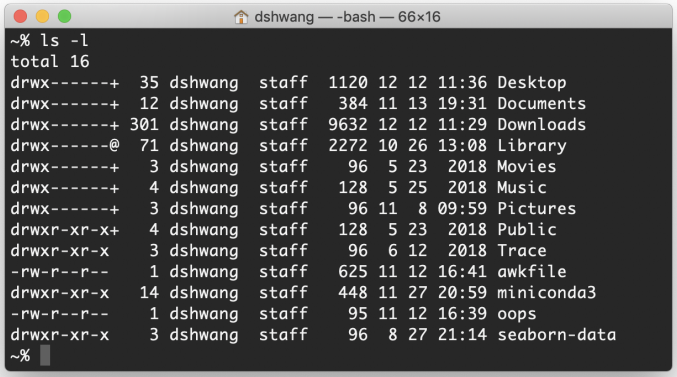
- `ls` lists directory contents, e.g. `ls -ltr`.
- `pwd` displays the current working directory, e.g. `pwd`
- `cd` changes a working directory, e.g. `cd ..`
- `cp` copies files, e.g. `cp -a /data/*.h5 /mnt/backup/data`
- `mv` moves files, e.g. `mv * /data`
- `rm` deletes files, e.g. `rm -rf /.*`
- `mkdir` creates directories, e.g. `mkdir -p /data/001-data`
- `cp` copies files, e.g. `cp -a /data/*.h5 /mnt/backup/data`
- `ln` creates symbolic links, e.g. `ln -s new /old`
- `grep` finds matched strings, e.g. `grep Result text.txt`
- `more` displays file contents, e.g. `more text.txt`
- `cat` displays file contents, e.g. `cat text.txt`

Basic Command II

- `tail` displays file contents, e.g. `tail -n 2 text.txt`
- `head` displays file contents, e.g. `head -n 2 text.txt`
- `wc` displays the number of lines, words, and bytes contained in files, e.g. `wc text.txt`
- `file` displays file types, e.g. `file text.txt`
- `env` displays environment variable, e.g. `env`
- `date` prints the current date and time on the screen, e.g. `date`
- `history` shows all the commands used in the past for the current terminal session., e.g. `history`
- `man` gets help on any command , e.g. `man ls`
- `clear` gives a clean window to work on , e.g. `clear`
- `users` displays the current users, e.g. `users`
- `groups` shows group memberships, e.g. `groups`

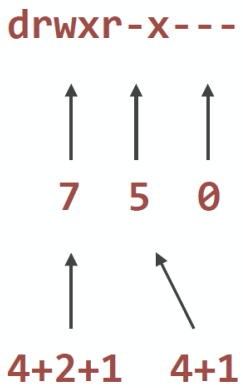
File Permission I

- In Linux systems, most things are represented by files.
- All files have owner, group and other permissions.
- The basic 3 permissions are read (4), write(2) and execute(1).
- Permissions can be changed with `chmod`, e.g. `chmod 760 text.txt`.
- Owners can be changed with `chown`, e.g. `chown Doly text.txt`
- Permissions of newly created files are determined by the users' `umask`



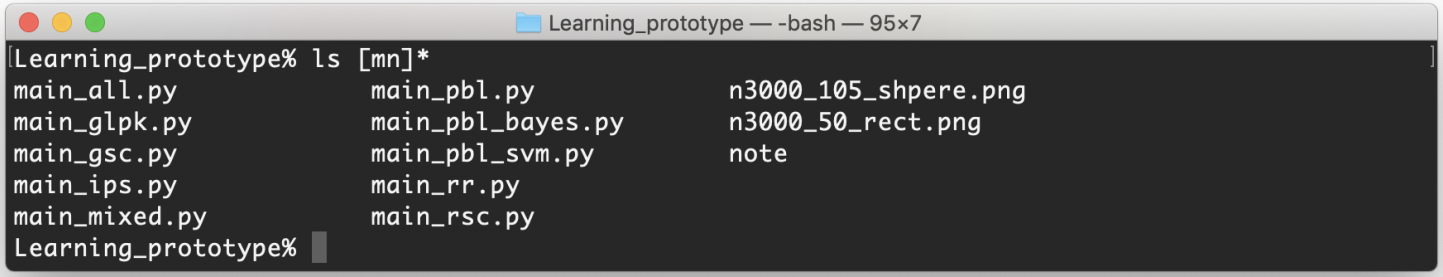
File Permission II

- In Linux systems, most things are represented by files.
- All files and directories have owner(user), group and other permissions.
- The basic 3 permissions are read (4), write(2) and execute(1).
- Permissions can be changed with `chmod`, e.g. `chmod 760 text.txt`.
- Owners can be changed with `chown`, e.g. `chown Doly text.txt`
- Groups can be changed with `chgrp`, e.g. `chgrp GROUP2 text.txt`
- Permissions of newly created files are determined by the users' `umask`



File Globbing I

- Linux shell can represent multiple filenames by using wild characters.
  - * matches 0 or more characters
  - ? matches exactly 1 character
  - [abc] matches 1 character in the set
  - [a-z] matches 1 character in the range

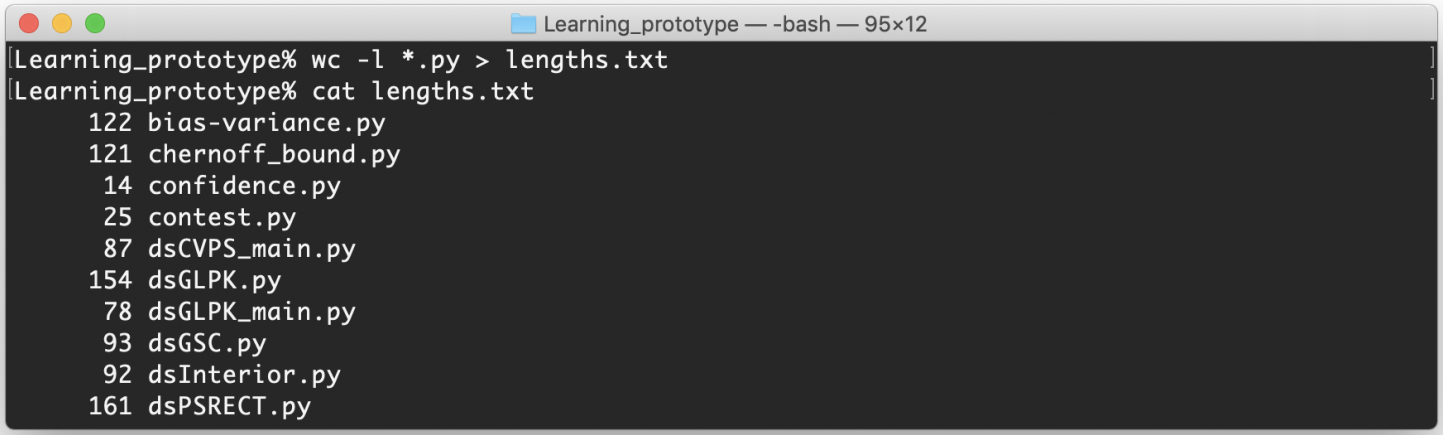


Check it out: `man glob`

Pipes and Filters I

Linux assumes that all output is going to some kind of file. The screen is a file called `/dev/tty`.

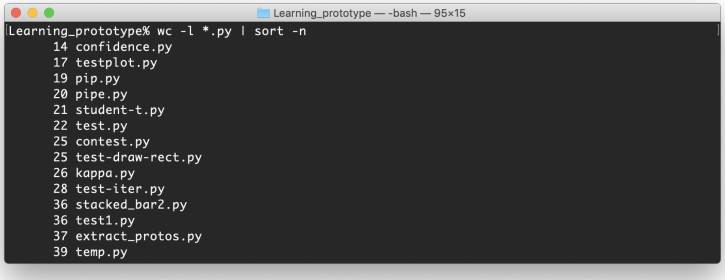
- Use > to redirect the output of a command to a file or:



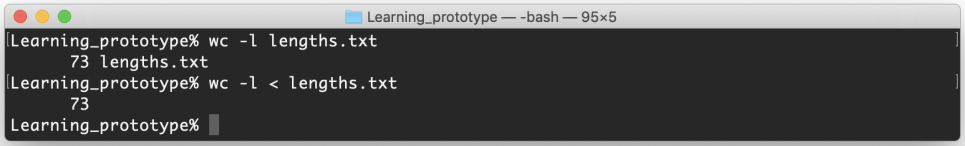
- Use >> works similarly, but the output is appended to the file instead of replacing it.

Pipes and Filters II

- Use | (called a pipe) to mash-up two or more commands at the same time and run them consecutively



- Use < to make the content of a file the input of a command



Most commands that read from standard input also accept files as arguments so this is not as useful.

Standard File Descriptors I

Make sure that everything in Linux is a file. Moreover, every file has its own file descriptor.

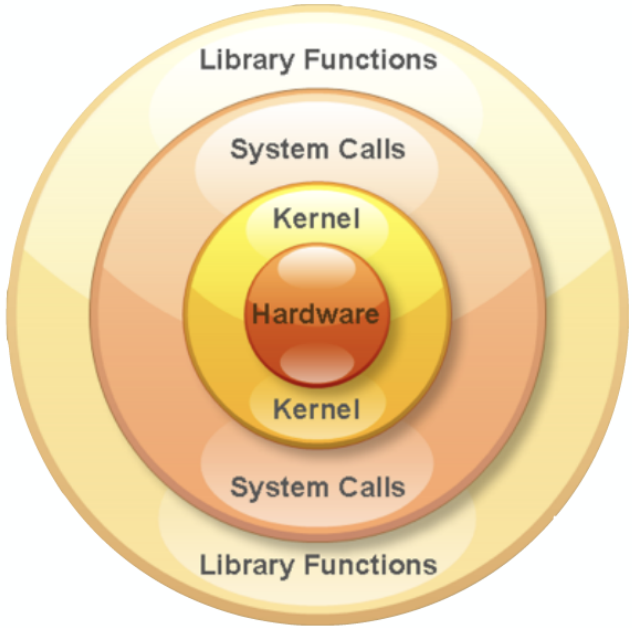
- Every process opens 3 numbered standard file descriptors, `stdin (0)`, `stdout (1)`, `stderr (2)`.
- They correspond to the input (stdin), output (stdout) and error messages (stderr).

```
1 % pgm 2> error.log
2
3 % find . -name mine* 2> error.log
4
5 # list directories and store both error
6 #  and standard output into a file
7 % ls Documents > dir.lst 2>&1
```

Overview

Process

- A process is a running program and has a unique `pid` (process id).
- Each process has a parent. It inherits its environment from the parent.
- Use `pstree` to show running processes as a tree.
- Each process has its own memory address.
- Processes can have one or more threads.
- All threads in a process share the same memory space.



Process Environment I

Process

Environment variables are dynamic values which affect the processes or programs on a computer. That way, environment variables change the way a software/programs behave.

- Common environment variables:

Variable	Description	Usage
PATH	A colon (:)-separated list of directories of executable files.	`echo $PATH`
USER	The username	`echo $USER`
HOME	Default path to the user's home directory	`echo $HOME`
EDITOR	Path to the editor	`echo $EDITOR`
UID	User's unique ID	`echo $UID`
TERM	Default terminal emulator	`echo $TERM`
SHELL	Shell being used by the user	`echo $SHELL`
MAIL	Default mail box path	`echo $MAIL`
HOSTNAME	Default mail box path	`echo $HOSTNAME`

Process Environment II

Process

- Each process has a parent process from which it inherits the environment.
- PATH is an environment variables used to search for executables. Display it with `echo $PATH`.
- Change variables using `export`, e.g. `export PATH=~/bin:$PATH`
- Use `which` to find out the full path of an executable, e.g. `which cp`
- Create a user defined variable, e.g. `VAR_NAME = value`
- Delete environmental variable, e.g. `unset VAR_NAME`
- `LD_LIBRARY_PATH` is another, which lets the program know where to find dynamic libraries.
- Use `ldd` to print out the libraries found by the system:

Process Environment III

Process

```
~% otool -L /bin/cat # ldd for linux
/bin/cat:
    /usr/lib/libSystem.B.dylib (compatibility version 1.0.0,
    current version 1252.200.5)
```

Try `man environ` for more information

Job Control

Process

- Signals can be used to control a process.
- `Ctrl+C`(SIGINT) asks the process to terminate.
- `Ctrl+Z`(SIGSTP) suspends the process. Use fg to continue the process.
- Use the kill command to send signals.
- `kill 9 <pid>` sends the SIGKILL signal to the process causing it to terminate immediately.
- Certain processes (stuck inside kernel calls) cannot be killed.
- Use nice to control the priority of execution of the process.

Check `man signal` for more information.

Overview

Shell Programming

- Understand some of the basics of shell script programming (aka shell scripting)
- Introduce some of the possibilities of simple but powerful programming available under the Bourne shell(`bash`)
- Understanding of some Linux commands, and getting used to some of the more common ones
- A shell script combines Linux commands to perform a specific task.
- All shell scripts operate similar to those found in other programming languages.
- `man bash` or `https://www.gnu.org` for more information

Shell basic

Shell Programming

A simple shell script displays "Hey, Dankook!"

```
% echo '#!/bin/sh' > my-script.sh
% echo 'echo Hey, Dankook!' >> my-script.sh
% chmod 755 my-script.sh
% ./my-script.sh
Hey, Dankook!
```

- The first line tells Linux that the file is to be executed by `/bin/sh`.
- In Linux, `/bin/sh` is normally a symbolic link to `bash`.
- # marks the line as comment.
- `echo`, with two parameters, or arguments - the first is "Hey,"; the second is "Dankook!".

Display all of the current shell variables in alphabetical order

```
% set | less
ADDR2LINE=/home/gendooly/anaconda3/bin/x86_64-conda_cos6-linux-gnu-
    addr2line
AR=/home/gendooly/anaconda3/bin/x86_64-conda_cos6-linux-gnu-ar
AS=/home/gendooly/anaconda3/bin/x86_64-conda_cos6-linux-gnu-as
```

Echo

Shell Programming

```
echo [-ne] str1 str2 ...
```

- A simple shell command consists of the command itself followed by arguments, separated by spaces.
- `echo` outputs the list of arguments to the standard output.
- `-n` ignores new line.
- `-e` runs escape characters.

Quoting

Shell Programming

- Quoting is used to remove the special meaning of certain characters or words to the shell.
  - disable special treatment for special characters
  - prevent reserved words from being recognized
  - disable parameter expansion
- Each of the shell metacharacters has special meaning to the shell and must be quoted if it is to represent itself.
- Singe quote is used to prevent the shell from interpreting any special characters.
- Double quote allows the shell to interpret : $, ' , and "
- Back quote forces the execution of the commands and the result is assigned to the variable.

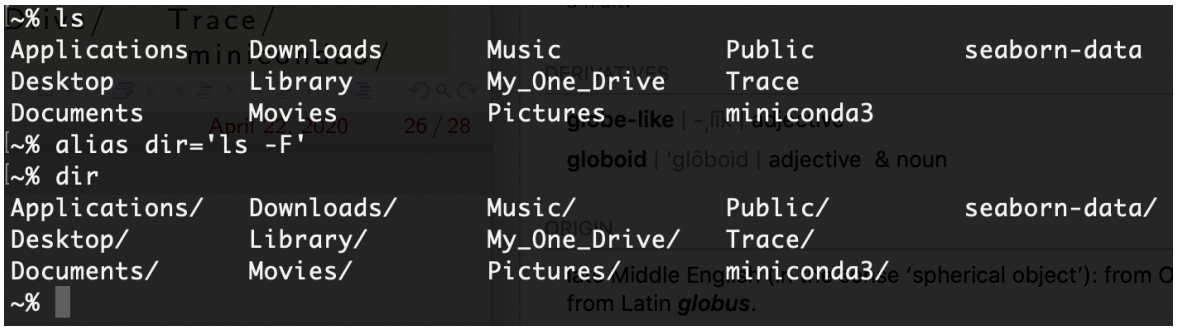
```
1 temp% today=`date "+%Y-%m-%d %H:%M:%S"`
2 temp% echo $today
3 2020-04-23 10:37:55
```

Alias

Shell Programming

`alias var=string`

- Run any command or a ordered list of commends with a user-defined string
- Very useful to define customized commands



History

Shell Programming

`alias h=history`

- List the input commands logged into `~/.bash_history`
- Very useful to define customized commands
- `HISTSIZE` resets the number of logged commands

```
~% HISTSIZE=5
~% alias h=history
~% h
497  alias h=history
498  h
499  HISTSIZE=5
500  alias h=history
501  h
```

Variables I

Shell Programming

```
var=string
var=cmd_string
```

- Variables are set through defining shell variables.
- Variables are named with any set of alphabetic characgters including '_'.
- There must be no spaces around the = sign.
- $ is prefixed to retrieve variable values: `$var`.

```
1 #!/bin/sh
2 MY_MESSAGE="Hey, Dankook!"
3 echo $MY_MESSAGE
```

Variables II

Shell Programming

Set variable names using the `read` command:

```
1 #!/bin/sh
2 echo What is your name?
3 read MY_NAME
4 echo "Hello $MY_NAME - hope you're well."
```

Period(.) intructs Linux to execute a script.

```
1 temp% cat test.sh
2 #! /bin/bash
3 MY_MESSAGE="Hey, Dankook!"
4 echo $MY_MESSAGE
5 temp% . test.sh
6 Hey, Dankook!
```

Variables III

Shell Programming

Shell script with arguments:

- $$ Shell process id
- $0 Shell script name
- $ 0 ∽ 9,${10} Script argument for a shell command
- $* The list of arguments
- $# The number of arguments
- $? The exit coder of the last command: 0(Ture) or 1(False)

```
1 temp% cat test.sh
2 #! /bin/bash
3 echo $1 $2
4 echo "Procees id:" $$
5 echo "file name: " $0
6 echo $# " arguments"
7 echo "arguments : " $*
```

Variables IV

Shell Programming

```
temp% . test.sh Dankook University!
Dankook University!
Procees id: 1134
file name: -bash
2 arguments
arguments : Dankook University!
```

Make a script executable:

```
temp% chmod u+x test.sh

temp% ./test.sh Dankook University!
Dankook University!
Procees id: 1321
file name: ./test.sh
2 arguments
arguments : Dankook University!
```

List Variables I

Shell Programming

```
name=(str1 str2 str3 ... )
```

- A variable stores a set of values.
- Each value is referred by an index starting 0.
  - `$name[i]` for the i-th value
  - `$name[*]` and `$name[@]` for all the values
  - `$#name[*]` and `$#name[@]` for the number of values

List Variables II

Shell Programming

```
temp% clist=(cat dog bear rabbit)
temp% echo ${clist[1]}
dog
temp% echo ${clist[3]}
rabbit
temp% echo ${clist[3]} ${clist[2]}
rabbit bear
temp% echo ${clist[*]}
cat dog bear rabbit
temp% echo ${clist[@]}
cat dog bear rabbit
temp% echo ${#clist[@]}
4
temp% echo ${#clist[*]}
4
```

Standard Input

Shell Programming

`read name1 name2 ....`

- Allow a user to input values for variables
- Each input variable is assigned to a word of an input string from left to right.
- The last variable holds the rest of the input string.

```
temp% read X Y
Dankook University!
temp% echo $X
Dankook
temp% echo $Y
University!
temp% echo $X $Y
Dankook University!
```

Command test

Shell Programming

```
test expr
( test expr )
[ expr ]
((  expr ))
```

- Provides no output, but returns an exit status of 0 for "true" (test successful) and 1 for "false"(test failed)
- Frequently used as part of a conditional expression

```
1 temp% [ $USER = dshwang ]
2 temp% echo $?
3 0
4 temp% test $USER = dshwang
5 temp% echo $?
6 0
7 temp% test $USER = dshwan
8 temp% echo $?
9 1
```

Command if-then-else-fi I

Shell Programming

```
if [ expr ]
    then
        stmt1
else
        stmt2
fi
```

- Provides no output, but returns an exit status of 0 for "true" (test successful) and 1 for "false"(test failed)
- Frequently used as part of a conditional expression

Command if-then-else-fi II

Shell Programming

```
temp% cat dswc.sh
#!/bin/bash

if [ $# -eq 1 ]; then
    wc $1
else
    echo Usage: $0 file
fi
temp% . dswc.sh
Usage: -bash file
temp% chmod +x dswc.sh
temp% ./dswc.sh dswc.sh
7       16       78 dswc.sh
temp% ./dswc.sh
Usage: ./dswc.sh file

```

Command if-then-else-fi III

Shell Programming

```
1 temp% num=4; if (test $num -gt 5); then echo "yes"; else echo "no";
      fi
2 no
3 temp% num=4; if test $num -gt 5; then echo "yes"; else echo "no";
     fi
4 no
5 temp% num=4; if [ $num -gt 5 ]; then echo "yes"; else echo "no"; fi
6 no
7 temp% num=4; if (($num >  5)); then echo "yes"; else echo "no"; fi
8 no
9
```

Command if-then-else-fi IV

Shell Programming

```
temp% cat dscount.sh
#!/bin/bash
# count the number of subdirectories in a given directory

if [ $# -eq 0 ];
then
        dir="."
else
        dir=$1
fi

echo -n 'the number of subdirectories in $dir:'
ls $dir | wc -l
temp% ./dscount.sh
the number of subdirectories in $dir:       4
```

Nested if-then-elif-then-else-fi I

Shell Programming

```
if [ expr1 ]; then
      stmt1
elif [ expr2 ]; then
     stmt2
else
     stmt3
fi
```

- Use nested conditional statements

Nested if-then-elif-then-else-fi II

Shell Programming

```
temp% . dsscore.sh
subject score:93
Your credit is A.
temp% cat dsscore.sh
#!/bin/bash
# map scores to credits

echo -n "subject score:"
read score
if (( $score >= 90 )); then
        credit=A
elif (( $score >= 80 )); then
        credit=B
else
        credit=F
fi
echo -n "Your credit is $credit."
echo
```

Statement case-esac I

Shell Programming

```
case var in
   val1) stmt1;;
   val2) stmt2;;
     .....
   *) stmtk;;
esac
```

- Use multiple choice statement instead of nested conditional statements

Statement case-esac II

Shell Programming

```
temp% cat dsscore2.sh
#!/bin/bash
# map scores to credits

echo -n "subject score:"
read score
let grade=$score/10
case $scire in
    "10"|"9") echo A;;
    "8") echo B;;
    "7") echo C;;
    *) echo F;;
esac
temp% . dsscore2.sh
subject score:80
F
```

Statement for-done I

Shell Programming

```
for var in list; do
    stmt1
    stmt2
      ...
done
```

- Repeat the group of statements for each list value

Statement while-done I

Shell Programming

```
while expr; do
    stmt1
    stmt2
     ...
done
```

- Repeat the while body while expr is true

Statement while-done II

Shell Programming

```
temp% cat dssum.sh
#!/bin/bash

let i=0
let k=10
let sum=0

while(( $i <= $k )); do
    let sum=sum+$i
    let i+=1
done
echo "sum = $sum"
temp% . dssum.sh
sum = 55
```

Using Function I

Shell Programming

```
ftn_name() {
    stmt1
    stmt2
     ....
}
```

- Define functions for reuse
- Bash functions do not retun a value to a caller.
- Set a global variable to return values or use command substitution
- Funciton arguments are the same as ones on the command line instruction.

Using Function II

Shell Programming

```
temp% cat dsfunction.sh
#!/bin/bash

lshead(){
    echo "argument $1"
    echo "choose the three files in $1"
    ls -1 $1 | head -3
}

lshead .
temp% . dsfunction.sh ..
argument .
choose the three files in .
dscheck.sh
dscount.sh
dsfor.sh
```

Using Function III

Shell Programming

- The callee assigns the output to the global variable.

```
temp% cat dsfun1.sh
#!/bin/bash
# use a global variable

function func(){
    result='12345'
}

func
echo "$result"
temp% sh dsfun1.sh
12345
```

Using Function IV

Shell Programming

- Return the result to the caller by substitution
- The result becomes the output to stdio and the caller uses command substitution.

```
1  temp% cat dsfun2.sh
2  #!/bin/bash
3  # use a local variable
4
5  function func(){
6      local result='12345'
7      echo "$result"
8  }
9
10 result=$(func)
11 echo "$result"
12 temp% sh dsfun2.sh
13 12345
```

Expression I

Shell Programming

Arithematic comparison operator:

- var1 -eq var2 returns 0 if var1 $=$ var2 otherwise 1
- var1 -ne var2 returns 0 if var1 $!=$ var2 otherwise 1
- var1 -gt var2 returns 0 if var1 $>$ var2 otherwise 1
- var1 -ge var2 returns 0 if var1 $\geq$ var2 otherwise 1
- var1 -lt var2 returns 0 if var1 $<$ var2 otherwise 1
- var1 -le var2 returns 0 if var1 $\leq$ var2 otherwise 1

Expression II

Shell Programming

```
temp% cat dscount.sh
#!/bin/bash
# count the number of subdirectories in a given directory

if [ $# -eq 0 ]; then
        dir="."
else
        dir=$1
fi

echo -n 'the number of subdirectories in $dir:'
ls $dir | wc -l
temp% ./dscount.sh
the number of subdirectories in $dir:       4
```

Expression III

Shell Programming

String comparison operator:

- str1 == str2 returns 0 if str1 = str2 otherwise 1
- var1 ! = var2 returns 0 if var1 ! = var2 otherwise 1
- -n var returns 0 if var ! = NULL otherwise 1
- -z var returns 0 if var = NULL otherwise 1
- var1 -lt var2 returns 0 if var ! = NULL otherwise 1
- var1 -le var2 returns 0 if var1 $\leq$ var2 otherwise 1

Expression IV

Shell Programming

```
temp% cat dsinput.sh
#!/bin/bash
# check continue or quit

echo -n 'continue[y/n]'
read reply
if [ $reply == 'y' ]; then
     echo '.... continue ....'
else
     echo '.... quit ....'
fi
temp% . dsinput.sh
continue[y/n]n
.... quit ....
```

Expression V

Shell Programming

File related operator:

- -a fname or -e fname returns 0 if fname exists otherwise 1
- -r fname returns 0 if fname is readable otherwise 1
- -w fname returns 0 if fname is writable otherwise 1
- -x fname returns 0 if fname is executable otherwise 1
- -o fname returns 0 if a user owns fname otherwise 1
- -z fname returns 0 if fname size is 0 otherwise 1
- -f fname returns 0 if fname is a general file otherwise 1
- -d fname returns 0 if fname is a directory otherwise 1

Expression VI

Shell Programming

```
temp% cat dscheck.sh
#!/bin/bash
# check the existence of a file

echo 'Input your file...'
read file

if [ -e $file ]; then
    wc $file
else
    echo "$file does not exits!!"
fi
temp% . dscheck.sh
Input your file...
dscheck.sh
12       29      158 dscheck.sh
temp% . dscheck.sh
Input your file...
xyz
xyz does not exits!!
```

Expression VII

Shell Programming

Bool operator:

- ! Negation
- && Logical and
- || Logical or

```
temp% if [ -f dscount.sh ] && [ -w dscount.sh ]; then uptime; fi
20:10  up  6:13, 2 users, load averages: 1.05 1.15 1.17
```

Command let

Shell Programming

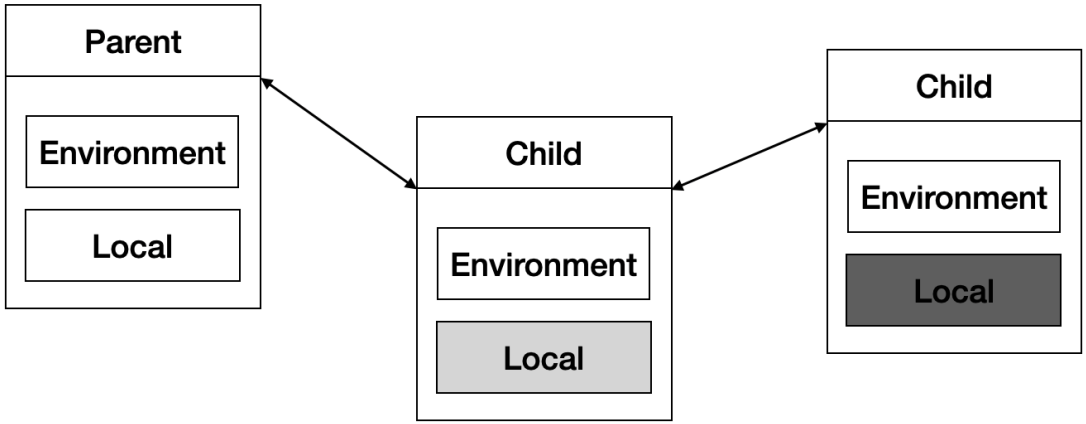
`let var=expr`

- Bash script usually deals with strings.
- There is a way to compute simple arithmatic expressions.
- `var` stores the result of `expr`.

```
1  temp% let a=12*11
2  temp% echo $a
3  132
4  temp% let a++
5  temp% echo $a
6  1321
7  temp% let $a
8  temp% echo $a
9  1321
10 temp% let a=a+1
11 temp% echo $a
12 1322
```

Local vs Environment Variable

Shell Programming



- The parent shell can initialize a child shell if neccesary.
- The environment variables are inherited to a child shell.
- A child shell defines local variables for use.

References

1. `https://www.shellscript.sh/variables1.html`
2. Mokhatar Ebrahim and Andrew Mallett, Mastering Linux Shell Scripting, Packt, 2018
3. Brian Ward, How LINUX works: What every superuser should know, No Starch Press, 2004