SYSTEMS DEVELOPMENT FOR COMPUTATIONAL SCIENCE

LECTURE 3

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LAST TIME

- More on Linux commands and the man-pages
- Unix philosophy and pipes
- Regular expressions and grep
- File attributes and the find command
- Text editors and IDEs

TODAY

Main topics: Command line customization, I/O redirection, Environment variables and shell scripting, Process management

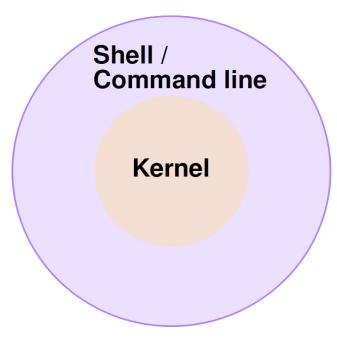
Details:

- Configuration files read by the shell at startup.
- Login shells and non-login shells.
- Redirection of file content and stdout/stderr.
- How to use environment variables and how to set them.
- Basics of writing shell scripts (same as typing commands in the shell but written in a file instead).
- Managing Jobs and processes in Linux, suspending and continuing execution.

LAB SECTIONS AND OFFICE HOURS

- You have been assigned to lab sections based on your preferences.
 You should have received an email notification if you submitted your preferences.
- Please check https://my.harvard.edu/ for your assigned lab section.
- If you were not assigned a lab section, please contact the teaching staff at cs107-staff@g.harvard.edu as soon as possible.
- You can find spreadsheets for time and location overview of office hours and lab sections in the class repository:
 - https://code.harvard.edu/CS107/main/blob/master/office_hours.xls
 - https://code.harvard.edu/CS107/main/blob/master/lab_groups.xls

RECALL THE SHELL IS YOUR COMMAND INTERFACE



- The tools of a carpenter are *essential* for his/her craft. They must be *sharp* for best results.
- Similar, the shell and editor are your tools. Make them your own.
- There are different shell interpreters:
 - sh (Bourne shell)
 - bash (Bourne Again Shell, Mac: since OSX Jaguar)
 - csh (C-shell)
 - ksh (Korn shell)
 - zsh (Mac: since OSX Catalina)
- Each of those shells executes a number of files at startup. You can use these files to run commands (rc) and configure your shell.

- Examples for configuration: user prompt, environment variables, auto-completion, command aliases, color theme and appearance, message of the day (motd), ...
- The configuration is implemented in startup files that are read by the bash shell whenever it starts. There are two types of shells which read the following files in the given order:
 - Interactive login shell or with --login option:
 - 1. /etc/profile
 - 2. ~/.bash_profile (if it exists, read and execute then stop)
 - 3. ~/.bash_login (if it exists, read and execute then stop)
 - 4. ~/.profile (if it exists, read and execute then stop)
 - Interactive non-login shell (e.g. a terminal emulator like xterm):
 - 1. ~/.bashrc

- Which files being read at shell startup depend on the shell you are using.
 See https://en.wikipedia.org/wiki/Unix_shell#Configuration_files for a good overview.
- Think of a *login shell* this way:
 - It is the first shell started when you login to the system. It must exist.
 - If you use Ubuntu with a GUI, you will not notice the login shell as the system boots directly into graphical mode.
 - On a headless server you will be dropped into a login shell. This is called an *interactive login shell*.
 - From the login shell you can create other shell instances, these are *interactive non-login* shells.

Summary for bash:

- Files read for interactive login shell:
 - 1. /etc/profile
 - 2. One of (in that order): ~/.bash_profile, ~/.bash_login, ~/.profile
- Files read for interactive non-login shell:
 - 1. ~/.bashrc

Typically, ~/.bash_profile contains this code:

```
1 [[ -f ~/.bashrc ]] && source ~/.bashrc # if ~/.bashrc exists, source its contents
```

Conclusion: to customize your bash shell, edit ~/.bashrc. To customize your zsh shell, edit ~/.zshrc instead.

Further information for startup files:

https://www.gnu.org/software/bash/manual/html_node/Bash-Startup-Files.html

A few comments about bash and zsh:

- Mac users will most likely be working with zsh, a newer shell with some additional features.
- The default shell on Linux is bash. You must install zsh from the package repo if you want to use it on Linux.
- While startup files may be different, most *scripts* should run with either shell.
- You will be confronted with bash on most remote machines and servers.
 Keep that in mind when you work with zsh and must be compatible with bash.

Additional reading for Mac users:

- Moving to zsh Scripting OSX
- What should/shouldn't go in .zshenv, .zshrc, .zlogin, .zprofile, .zlogout?
- About .bash_profile and .bashrc on MacOS

Simple . bashrc example:

- A useful adaptive prompt for bash and zsh: https://github.com/nojhan/liquidprompt
- Shell color themes based on 16 colors: https://github.com/chriskempson/base16-shell
- There are many more online to be found via search engines.

EXAMPLES FOR SHELL CUSTOMIZATION

- You find yourself often typing 1s -1. Create an *alias* named 11 to minimize your future typing overhead. (See previous slide for an example alias.)
- Figure out what the prompt from the previous slide is doing:

```
1 # set a custom primary prompt: promt is defined in the variable PS1, see `man bash`
2 export PS1='\e[36m\w\e[0m\$'
```

Configure your own prompt. This page might be helpful.

Change the interpretation mode to vi with

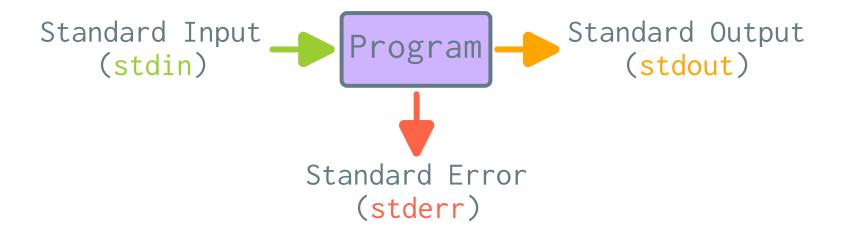
```
$ set -o vi
```

Your shell now operates with *normal* and *insert* modes, similar to vi or vim. You can change back to non-modal interpretation with

```
$ set -o emacs
```

which is the default.

INPUT/OUTPUT (I/O) AND REDIRECTION



- Inside the shell, stdin is received from your keyboard
- A program generates two output streams:
 - 1. stdout: normal program output
 - 2. stderr: output associated to something gone wrong (e.g. compiler warning or error)
- Recall the file descriptors: stdin=0, stdout=1, stderr=2
- To send and EOF (end-of-file) character, press ctrl-d

REDIRECTION OF I/O STREAMS

- You have learned about the Unix pipe "|" which redirects the stdout of a program into the stdin for the next program in the pipeline (see the "SHELL GRAMMAR" section in man bash)
- You can also redirect any data stream to or from files.
- To redirect stdout to a file use the ">" operator:

```
$ ls -l > ls_long_output # redirect output into file
```

To redirect file contents to stdin use the "<" operator:

```
$ sort < some_data # input content of some_data into sort</pre>
```

You can combine both:

```
$ sort < some_data > some_sorted_data
```

Or equivalently using a pipe (the above is more compact)

```
$ cat some_data | sort > some_sorted_data
```

REDIRECTION OF I/O STREAMS

- You can either *create* (or overwrite) files or append to existing files:
 - Use > to create or overwrite (it will delete previous contents)
 - Use >> to append to existing files (ideal for logging)
- There are two special data sinks in Linux:
 - 1. /dev/null: data written to this device is *discarded*. Reading from this device always returns the end-of-file (EOF) character.
 - 2. /dev/zero: data written to this device is *discarded*. Reading from this device returns the '\0' (NUL) byte (see ASCII table).

Example: filter spam email and send it to /dev/null

\$ script_to_filter_spam_email >/dev/null # /dev/null behaves like a black hole

REDIRECTION OF I/O STREAMS

- File redirection operates on stdout by default.
- You can specify the *file descriptor* explicitly. **Example:** to redirect stderr use file descriptor 2:

```
$ my_prog 2> error_log # only redirect stderr
```

 For convenience, you can redirect both stdout and stderr at the same time using the "&" descriptor:

```
$ my_prog &> full_log # redirect stdout and stderr
```

• This also works if you want to use pipes (by default only stdout is piped into stdin):

```
$ prog1 | & prog2 # pipe stdout and stderr into stdin of prog2
```

You can also chain redirection operators:

```
$ my_prog > my_output 2> my_error_log # write error log file
$ my_prog > my_output 2>&1 # redirect stderr to stdout instead of separate file
```

ASIDE: WHITE SPACE IN FILENAMES

 We have seen the wildcard "*" that matches every character (even white space). For example: list all python files

```
$ ls
exercise_1.py exercise_2.py README.md
$ ls *.py
exercise_1.py exercise_2.py
```

• White space in filenames: although common on Windows, it is bad practice to create filenames with spaces. In the shell, white space separates arguments to commands and you must take special care when you parse filenames. Example:

```
1 $ touch exercise 1.py; ls # touch creates 2 files: 1.py and exercise
2 1.py exercise README.md
3 $ touch exercise\ 1.py; ls # you must escape white space to get a single file
4 1.py exercise 'exercise 1.py' README.md
5 $ touch 'exercise 2.py'; ls # or pass a string
6 1.py exercise 'exercise 1.py' 'exercise 2.py' README.md
```

ENVIRONMENT VARIABLES

- You can customize your environment by setting the values of certain *environment variables*.
- You have already seen them when customizing your prompt by setting the value of PS1, which is an environment variable.
- You can get a list of all environment variables and their corresponding value with the env command
- Any shell variables (not only environment variables) can be dereferenced by prefixing them with a "\$" character:

```
$ my_var='Hello CS107/AC207!'
$ echo $my_var
Hello CS107/AC207!
$ echo my_var
my_var
$ echo $HOME # Environment variables are usually written in ALL CAPS
/home/fabs
```

THE PATH ENVIRONMENT VARIABLE

The role of the PATH environment variable is to specify the search path(s) used by the shell to find executable programs.

- For every command you enter, the shell checks if this command is a built-in command (see the "SHELL BUILTIN COMMANDS" in man bash).
- If it is not built-in, the shell will check the path(s) defined in the PATH environment variable to see whether it can find the executable in these locations.
- Finally, the shell will give up:

```
$ this_command_does_not_exist
bash: this_command_does_not_exist: command not found
```

• If a command is not reachable via PATH but the *path to the executable is* specified instead, the shell will execute the command (see lecture codes):

```
$ ./this_command_exists_locally # note the leading path `./`
You have executed ./this_command_exists_locally
```

THE PATH ENVIRONMENT VARIABLE

• By default, PATH holds at least the relevant paths for your *system commands* (e.g. /usr/bin). It is a good idea to extend it in your .bashrc as follows:

```
1 PATH=$HOME/bin:$HOME/.local/bin:$PATH
2 export PATH
```

- Each path specified in PATH must be *delimited* by a colon ":". This is true for any environment variable that holds a list of paths, e.g. MANPATH, INFOPATH, PYTHONPATH and others.
- The export keyword ensures that your customized PATH is available in other shell instances as well
- \$HOME/bin: a standard path in your home directory for executable scripts or programs
- \$HOME/.local/bin: default path used by python to install packages in a Linux user directory (some of those packages come with executables and you want to access them). *Example:* the command below installs a Python package "package_name" below your \$HOME/.local path by default:

```
$ python -m pip install --user <package_name>
```

THE PATH ENVIRONMENT VARIABLE

- 1 PATH=\$HOME/bin:\$HOME/.local/bin:\$PATH # note the last \$PATH expansion!
- 2 export PATH

Order is important:

- You must dereference the content of PATH in your re-assignment of PATH (see line 1 above) in order to keep what was previously defined in it.
- Append it at the end to ensure that your custom executables (with possibly the same names as already existing ones) take precedence!
- Once the shell has found a matching executable in PATH, it will not look any further.

Example: Assume you have the executables \$HOME/bin/my_exec and \$HOME/.local/bin/my_exec and your PATH is set as shown above. If you run

\$ my_exec

the executable in \$HOME/bin/my_exec will be executed.

SETTING SHELL VARIABLES

 You can omit the export keyword. In that case the variable will only be available in the current shell instance:

With export:

You must use export in your . bashrc or . zshrc files to ensure the settings propagate correctly.

You can delete any variable using the unset command:

```
$ my_var='Hello World!' # set a variable in the current shell
$ unset my_var # unset it again in the current shell
$ echo $my_var # my_var is empty
```

WHAT IS SHELL SCRIPTING?

- Typing out a series of commands that do complex tasks is not convenient and will only remain in your history for a short time.
- Shell scripting (and also Python scripts) is a powerful way to perform all kinds of *automation tasks*, often repetitive in time.
- By setting shell variables from the previous slides, you have already seen an important mechanism of shell scripting.

A shell script is an *executable file* that contains commands together with pipes, file redirection and structures such as loops or if-conditionals to perform (more complex) tasks in the command line. A shell script allows you to archive and *replay* the commands in the script. Such (user) scripts are often placed in \$HOME/bin and have permissions 700 (owner only) or 755 (group and others can read and execute as well).

SHELL SCRIPTING INTERPRETER

You should be specific about which shell (interpreter) you want to target in your scripts. This ensures *portability* of your scripts.

You specify the interpreter with a shebang. The general form is:

1 #!interpreter_command [optional arguments]

which you must write at the very beginning of your script.

• Examples are:

bash:	#!/usr/bin/env	bash
zsh:	#!/usr/bin/env	zsh
python:	#!/usr/bin/env	python3

Note: Use the /usr/bin/env command to resolve the actual path of the interpreter you target. Some users might have custom installations for these interpreters in their PATH. Hard-coding a path like /bin/bash, for example, would ignore this customization and possibly annoy users of your scripts.

SHELL SCRIPTING INTERPRETER

Your script *must be executable*, like any other program. By now you know how to do that. The following is an example script called my_exec (see lecture code):

```
1 #!/usr/bin/env bash
2 echo "I am script $0, running inside $PWD."
3 echo "The following arguments were given:"
4 for arg in "$0"; do
5    echo $arg
6 done
```

- Save the script inside \$HOME/bin because we have setup this path is in PATH. The suffix .sh is optional, you can choose any name you want. It is just a file.
- Set executable permissions and run it:

```
$ chmod 755 ~/bin/my_exec
$ pwd
/home/fabs
$ my_exec Hello World!
```

What output do you expect?

SHELL SCRIPTING SPECIAL VARIABLES

There are some special variables that you can make use of in your scripts and functions:

\$@	Expands to quoted arguments. For previous example: "Hello" "World!"
\$0	The full path of the script. (Always use \$0 for your help messages in case you rename your script later.)
\$1, , \$9	The first nine script arguments. For previous example: \$1 \rightarrow Hello and \$2 \rightarrow World!
\$#	The number of arguments passed to the script. For previous example: $\$\# \rightarrow 2$

A NOTE ABOUT STRINGS

Strings are very useful in scripts. They exist in two variants:

1. Hard-quoted strings: single-quotes

```
1 expansion=1234
2 str='This is a literal string, no variable ${expansion}' # single-quotes
3 echo ${str}

1 This is a literal string, no variable ${expansion}
```

2. Soft-quoted strings: double-quotes

```
1 variables='random values from other variables'
2 str="This string allows me to expand ${variables}" # double-quotes
3 echo ${str}
```

1 This string allows me to expand random values from other variables

SHELL SCRIPTING: for-LOOPS

Often you need to loop over a list of items obtained from another command invocation:

```
1 #!/usr/bin/env bash
2 dir=$1 # what does this line do?
3 for f in $(find $dir -maxdepth 1 -type f -name "*.py"); do
4  # f: iteration variable
5  # in: expects a list of items (for iteration)
6  echo $f # you would do something more meaningful here
7 done
```

The "\$(...)" executes the statement inside the parenthesis in a subshell and returns the stdout to the caller. You can use pipes for the commands in parenthesis as well. Such command substitutions are very useful in shell scripts and have numerous applications. Note: in the older Bourne shell, command substitutions were accomplished with backticks instead "`...`".

SHELL SCRIPTING: if-CONDITIONALS

The general form for an *if*-conditional looks like this:

```
1 if [ condition_A ]; then
2  # execute this block when condition_A is true
3 elif [ condition_B ]; then
4  # execute this block when condition_B is true
5 else
6  # execute this block otherwise
7 fi # except for loops, the end-delimiter of constructs is the construct name in
8  # reverse
```

Main reference for *if*-conditionals:

https://tldp.org/LDP/Bash-Beginners-Guide/html/sect_07_01.html

if-CONDITIONALS: STRING COMPARISONS

String comparison condition:

Examples: (see lecture codes)

if-CONDITIONALS: STRING COMPARISONS

Example: compare a string argument

```
1 #!/usr/bin/env bash
2 if [ "$1" == 'Hello CS107/AC207!' ]; then
3    echo 'Success!'
4 else
5    echo 'Got unexpected string argument'
6 fi
```

What output do you expect from the following invocation?

```
$ ./string_comparison.sh Hello CS107/AC207!
```

if-CONDITIONALS: INTEGER COMPARISONS

Integer comparisons: the general form is

[INT1 OP INT2]

where OP is one of the following:

```
-eq INT1 is equal to INT2
-ne INT1 is not equal to INT2
-lt INT1 is less than INT2
-le INT1 is less than or equal to INT2
-gt INT1 is greater than INT2
-ge INT1 is greater than or equal to INT2
```

See https://tldp.org/LDP/abs/html/comparison-ops.html

if-CONDITIONALS: INTEGER COMPARISONS

Example: integer comparisons

```
1 #!/usr/bin/env bash
2 if [ $# -gt 2 ]; then
3    echo "Number of arguments $# is larger than two"
4 else
5    echo "Number of arguments $# is less than or equal to two"
6 fi
```

Testing with different number of arguments:

```
$ ./int_comparison.sh a b
Number of arguments 2 is less than or equal to two
$ ./int_comparison.sh a b c
Number of arguments 3 is greater than two
```

if-CONDITIONALS: FILES AND DIRECTORIES

Often you need to test if files exist:

```
[ -d FILE ] True if FILE exists and is a directory

[ -f FILE ] True if FILE exists and is a regular file

[ -e FILE ] True if FILE exists

[ -r FILE ] True if FILE exists and is readable

[ -w FILE ] True if FILE exists and is writable

[ -x FILE ] True if FILE exists and is executable
```

Note that instead of FILE (which is some path to a file) you can also specify a file descriptor using <code>/dev/fd/n</code> with n the file descriptor ID. (recall: stdin=0, stdout=1, stderr=2, ...)

See: https://tldp.org/LDP/Bash-Beginners-Guide/html/sect_07_01.html

if-CONDITIONALS: FILES AND DIRECTORIES

Example: simple testing for files (file_check.sh)

```
1 #!/usr/bin/env bash
 2 if [ $# -ne 1 ]; then
       cat <<EOF
   USAGE: $0 <path/to/file>
       More documentation here. The form used here is called a here-document.
       They are very useful to write longer strings and expanding variables like
       \$0 above. See https://tldp.org/LDP/abs/html/here-docs.html
   E0F
       exit 1 # exit with failure code
  fi
12
   if \lceil -f \$1 \rceil; then
       echo "File $1 exists and is a regular file"
   elif [ -d $1 ]; then
       echo "File $1 exists and is a directory"
   elif [ -e $1 ]; then
       echo "File $1 exists and is an unknown file"
19 fi
```

You can find this example script in the lecture codes:

https://code.harvard.edu/CS107/main/tree/master/lecture/code/lecture03

SHELL SCRIPTING REFERENCE

- This the essential reference for bash scripting: https://tldp.org/LDP/Bash-Beginners-Guide/html/index.html
- More advanced topics: https://tldp.org/LDP/abs/html/index.html
- Writing scripts requires *practice*.
- When you notice that you keep repeating a task over and over, write a script instead and save it in ~/bin for example.
- bash scripts are extremely useful to automate tasks that involve batch processing. This may include filtering noise from data, generating movie frames, running periodic data backups or automating the submission of computing jobs on supercomputers.
- bash scripts are not very well suited for floating point arithmetic (use python for this).

JOB/PROCESS MANAGEMENT

Any process or job is assigned a unique PID:

```
$ sleep 100

$ ps aux | grep sleep # this is run in another bash instance, you see why in a second
fabs     145691 0.0 0.0 5364 688 pts/4 S+ 12:19 0:00 sleep 100
```

The PID for this sleep process is 145691

- The shell gives you some tools to manage such processes:
 - Run them in the background
 - Move a job to the foreground
 - Suspend a job
 - Terminate a job
- Running a process will block your prompt. The above command sleep 100 will return back control only after 100 seconds have passed.

RUNNING JOBS IN BACKGROUND

The shell returns control immediately by appending a "&"

• Appending a & will put the job in the *background*, you could exit the shell and the job would continue to run. (Only if the shell you are quitting is a *non-login shell*!)

SUSPENDING JOBS

• You can suspend a job to get back control of the shell by pressing Ctrl-z.

A stopped (or suspended) job *does not make progress*! If you want to quit the current shell (even if inside an interactive non-login shell) it will warn you the first time you try:

```
$ exit
exit
There are stopped jobs.
$ exit # the second time you call exit (or Ctrl-d) the shell will quit without warning
```

You can bring a stopped job back to foreground by using the fg command.

LIST JOBS AND PROCESSES

You can list and display running jobs and processes in several ways:

- jobs (see man jobs): displays the status of jobs in the current session (running, stopped, terminated)
- ps aux (see man ps): list all running processes on stdout. You may need to filter through grep to find what you are looking for.
- top (always available on Linux, see man top) to list a job ranking based on resource usage.
- Similar to top with better multi-core support: htop (see man htop). You may need to install it. In Ubuntu: sudo apt-get install htop
- Many others exists with more fancy presentation of data. For example https://github.com/cjbassi/ytop

TERMINATE JOBS

- You can terminate any job you have appropriate permissions.
- You can graciously terminate a job or forcefully kill it. (What would you prefer? (**)
- You should only use the latter
 when there is no hope. Example:
 system starts to become
 unresponsive due to memory leak.
- The former will make sure that claimed resources are freed correctly and child processes are shutdown first. Relevant for multithreaded programs.



TERMINATE JOBS

You terminate jobs by sending a signal through the kill command. See:

- By default kill will send a SIGTERM signal which is *graceful*. The rude one is called SIGKILL.
- You can specify the signal with the -s option of the kill command (be sure you get the PID right! Use ps or top to get it). **Example:**

```
$ kill -s SIGKILL <PID> # only do this when nothing else works anymore
```

• If you are sure that, for example, python is causing you trouble, you can send a SIGTERM by name using the killall command:

```
$ killall python
```

TERMINATE JOBS

• You terminate jobs by sending a *signal* through the kill command. See:

- You can send an interrupt signal (SIGINT) by pressing Ctrl-c
- A SIGINT can be *catched* and processed differently by interactive software. For example, a hanging Python script will not always terminate with Ctrl-c because the interpreter will catch the signal and decide what to do with it. Use killall python instead.
- In most of the cases a SIGINT translates to SIGTERM

RECAP

- Take advantage of the shell customization and adapt it to best suit your workflow.
- I/O redirection and pipes are powerful tools that you must internalize when you spend the majority of time in the shell
- Process management and suspension is important once you are in the role of system administration or if you need more fine grained control over your processes.
- Environment variables allow you to further customize your system. They are very powerful and can be (and should be) used in shell scripting

Further reading:

- Bash beginners guide: https://tldp.org/LDP/Bash-Beginners-Guide/html/index.html
- Advanced Bash scripting: https://tldp.org/LDP/abs/html/index.html
- Bash startup files: https://www.gnu.org/software/bash/manual/html_node/Bash-Startup-Files.html
- S. R. Bourne, "An Introduction to the UNIX Shell", Bell Laboratories (reading/bourne1997.pdf in main repository)
- S. R. Bourne, "The Unix Shell", Byte Magazine, 1983. Link