Welcome to the Advanced Unix Workshop!

Please sign into the LAS training server:

Mac/Linux users:

In terminal:

`ssh <your-net-id>@training.las.iastate.edu`

Windows users:

In PuTTY “hostname” box:

`<your-net-id>@training.las.iastate.edu`

Mac/Linux/Windows users, after sign-in:

`git clone https://github.com/cmmann/20181013-adv-unix.git`

Advanced UNIX

BCBGSO Workshop

October 13, 2018

Presenter: Carla Mann

Thanks!

- BIG thanks to Jennifer Chang for inspiration for slides and materials
- Organizers: Paul Villanueva and Basil Khuder
- Funding/Support/Volunteers: BCBGSO
- Tech support: Biology IT, especially Levi Baber

Huge thanks to our MANY BCBGSO student volunteers!

Materials

- All exercise activities from this workshop are available at:

https://github.com/cmmann/20181013-unix-adv

- Supporting materials are available at:

https://github.com/cmmann/20181013-UNIX-ADV-MATERIALS/

You can download this PowerPoint and follow along on your computer.

- You will probably benefit quite a bit from downloading (and using) the cheat sheet!

Sticky Notes

Write your name (in big letters) on BOTH sticky notes

If you need help, stick the MAGENTA sticky note to your laptop (or raise your hand)

If things are going well/you've completed an exercise, stick the GREEN sticky note to your laptop

Overview

Lesson 0: Quick Review of Basic Unix

Lesson 0.5: Setup

Lesson 1: Text Editing with `nano`

Lesson 2: Shell Scripting

Lesson 3: Loops

Lesson 4: Data Exploration with `grep`

Lesson 5: Regular Expressions (if we get to it)

Lesson 0: Quick Review

When describing a path to an/application:

```
this/is/path/to/the/file.txt
```

For our purposes:

- "folder" and "directory" refer to the same thing
- "terminal", "console", and "console window" all refer to the place you will type commands

In PowerPoint, commands you will type in the terminal will look `like this`

Keys you press will look like this: **[Ctrl]** or **[command]**

If you should press keys at the same time: **[Ctrl]** + **[C]**

A name or value that is user-dependent or variable will look `<like this>`

Don't use spaces in names; use dashes **[-]** instead

`cd`: change directory

`ls`: list directory contents

`man <command>`: show manual page for command

Set-Up

Mac/Linux:

Open terminal

```
ssh <your-netid>@training.las.iastate.edu
```

Windows:

Open Putty.exe

Enter

`<your-net-id>@training.las.iastate.edu`
into the Host Name box

Lesson 0.5: Setup

Once logged in, use this command to clone the materials into your workspace:

```
git clone
https://github.com/cmmann/20181013-unix-
adv.git
```

If you are prompted for a username/password, check to make sure you typed the URL correctly!

Lesson 1: Text Editing

Overview:

Lesson 1.1: Text Editors in UNIX

Lesson 1.2: `nano`

Lesson 1.1: Text Editors in UNIX

Multiple ways of editing text in files in UNIX

`Vim` is a VERY powerful text editor, but has a steep learning curve

- Very worthwhile to learn, but we could spend an entire workshop on it, so we're not going to mess with it today

"Friendliest" Unix text editor is `nano`

*If you already know how to use Vim, feel free to use it!

Lesson 1.2: Text Editing with nano

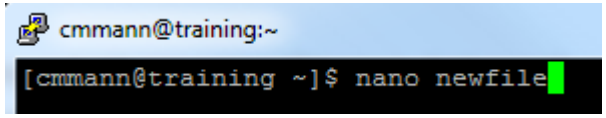
Command:

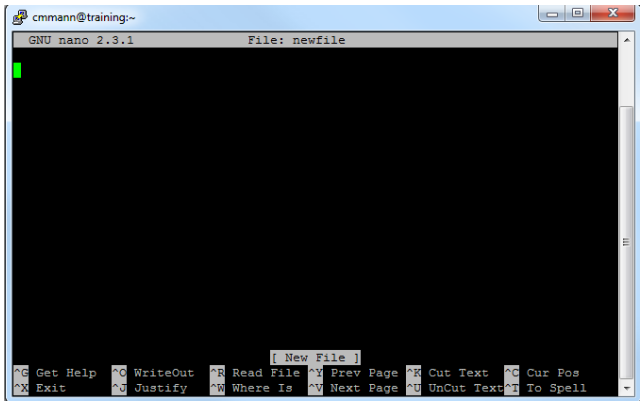
```
nano <filename>
```

What it does:

If `<filename>` exists, `nano` will open the file and you can read and manipulate it

If `<filename>` does not exist, `nano` will create a new file called `<filename>` and open it for you





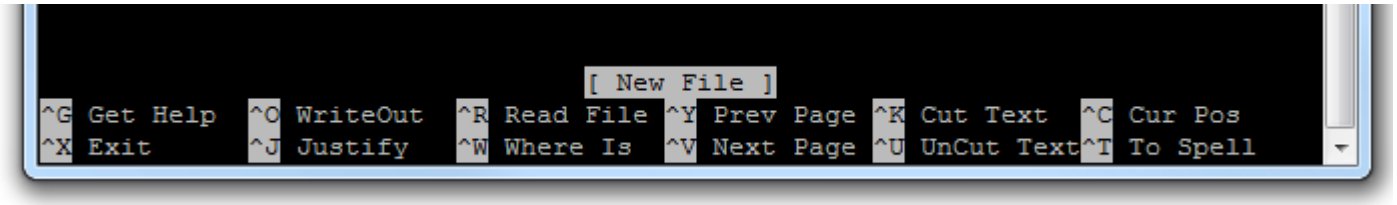
Lesson 1.2:
Text Editing with `nano`

`nano` is kind enough to give you a list of controls at the bottom of the editing window

You can easily type in the `nano` window just as you would in Notepad, TextEdit, or any other text editor

To exit out of a `nano` window, type **[Ctrl]+[x]**

`nano` will ask if you want to save changes; type **[y]** or **[n]**



Exercise 1:

Goals:

1. **Navigate** to `20181013-unix-adv/exercise1/`
2. Use **nano** to open "`exercise1.txt`"
3. **Edit** the text of "3. What is the capital of Assyria?" to read "3. What is your favorite color?"
4. Answer the questions in the file
   (the answers don't really matter, just your ability to edit the file)
5. **Exit** (save when prompted)

Exercise 1:

Goals:

1. Navigate to `20181013-unix-adv/exercise1/`
   `cd 20181013-unix-adv/exercise1`
2. Use nano to open "`exercise1.txt`"
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4. Answer the questions in the file
   (the answers don't really matter, just your ability to edit the file)
   ```
   Carla
   I seek the Holy Grail
   Blue
   An African or European swallow?
   42
   ```
5. Exit (save when prompted)

Exercise 1:

Goals:

1. Navigate to `20181013-unix-adv/exercise1/`
   ```
   cd 20181013-unix-adv/exercise1
   ```
2. Use nano to open "`exercise1.txt`"
   ```
   nano exercise1.txt
   ```
3. Edit the text of "3. What is the capital of Assyria?" to read "3. What is your favorite color?"
4. Answer the questions in the file
   (the answers don't really matter, just your ability to edit the file)
   ```
   Carla
   I seek the Holy Grail
   Blue
   An African or European swallow?
   42
   ```
5. Exit (save when prompted)
   ```
   [Ctrl]+[x]
   [y]
   ```

Lesson 2: Shell Scripting

Overview:

Lesson 2.0: What is a shell?

Lesson 2.1: Creating a shell script

Lesson 2.3: Executing a shell script

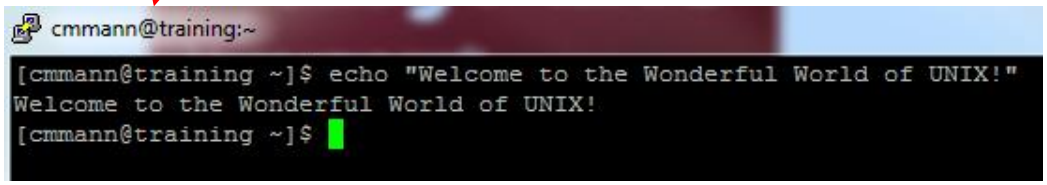
Exercise 2: Completed throughout the lesson

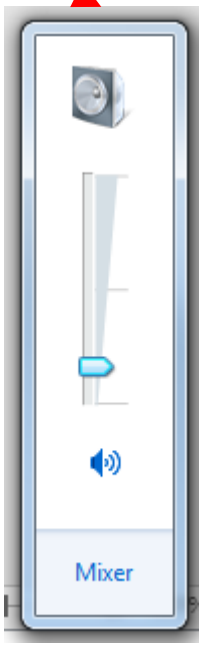
Lesson 2.0: What is a shell?

A shell is an interface for accessing an operating system's services

Shells can be GUIs (graphical user interface)

or CLIs (command-line interface)





Lesson 2.0: What is a shell?

There are multiple ‘flavors’ of command-line interfaces:

DOS, POSIX, CMD.EXE, many others

We are going to use a command-line shell called Bash:

To enable Bash scripting on your terminal, enter:

```
bash
```

And as simply as that, the server now knows what to use to interpret commands

Lesson 2.0: Shell Scripting

Every command you type into your terminal can be saved into a file

This file is called a *shell script*

That file can then be *executed*, or run, from the terminal

The commands in the file will be read line-by-line and executed, as if you had typed them in the terminal

Lesson 2.1: Creating a Shell Script

When creating a shell script, we first need to create a file

This file should end in ".sh", which signifies that it is a shell script

Note that the computer doesn't require the ".sh" extension to recognize this (it uses something different) – this is a human convention so you know the file contains a shell script

Exercise 2:

Create a file, using `nano`, called "`hello.sh`"

Lesson 2.1: Creating a Shell Script

WE know the script should be executed with `bash` – Unix doesn't.

How do we tell UNIX what tools to use?

By starting off the file with a hashbang and a file path!
This tells UNIX to use certain a certain shell to run the script

```
#!<path/to/program>
```

In our case, we're using bash. So the first line of `hello.sh`, and EVERY SHELL SCRIPT YOU WRITE (that will be interpreted with bash), will be:

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

Exercise 2: Go ahead and add this header to `hello.sh`

Lesson 2.1: Comments

Scripts can be complicated

Keep track of what scripts are doing with *comments*

In .sh files, any text following '#' is ignored by bash

#So this is ignored
But only #this last bit is ignored

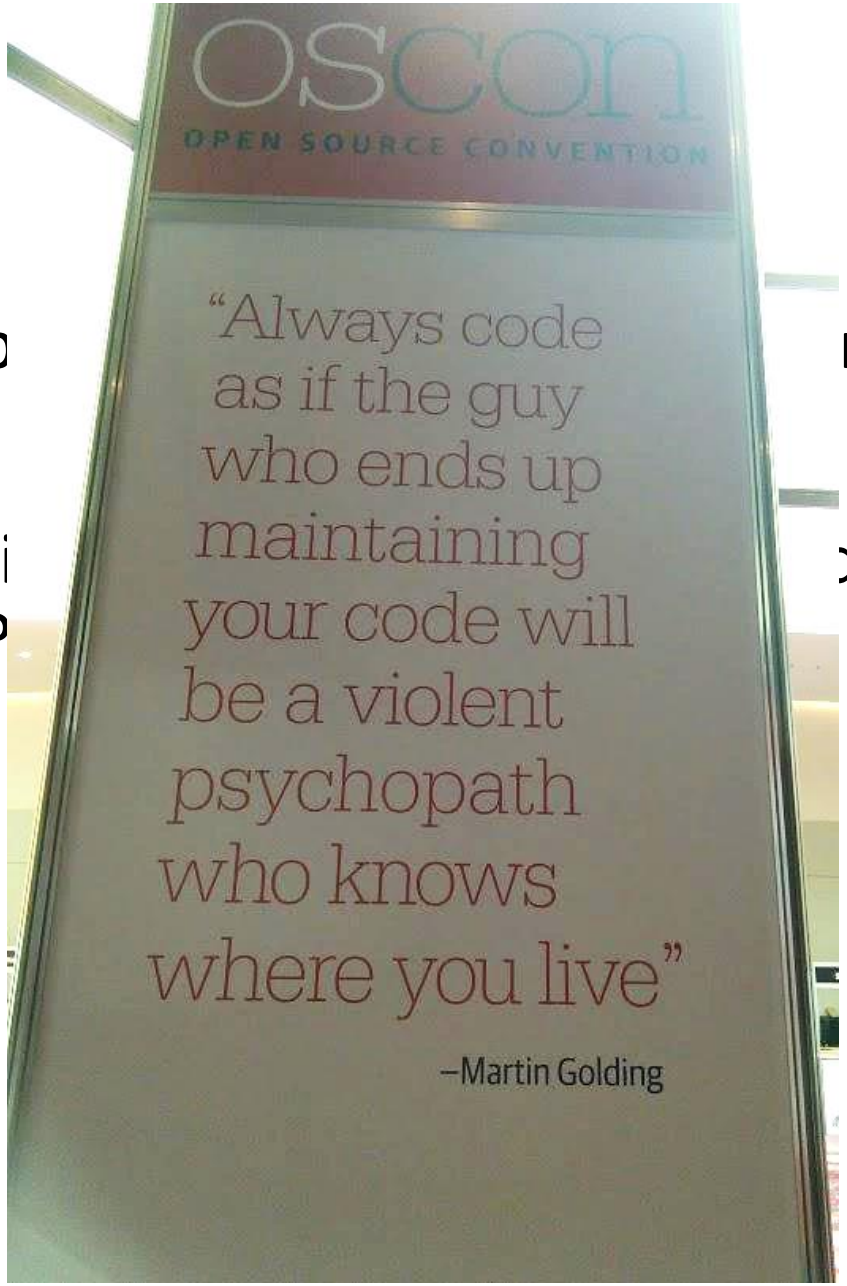
Exercise 2:

#Using a comment, add your name and the date to your `hello.sh` script

Lesson

It is good p ripts well

Will you sti doing 6 months from now?



Lesson 2.1: Creating a Shell Script

We are going to create a simple script within `hello.sh` that prints “hello” to the console upon execution.

You can print to the console using the command “echo”:

```
echo “what you want to say”
```

Lesson 2.1: Creating a Shell Script

You can do the same thing, within the script

Exercise 2:

In your hello.sh file, type:

```
echo "hello world!"
```

or

```
echo "Hello, world!"
```

(if you want to be grammatically correct)

Then exit and save the file.

Lesson 2.2:
Executing a Shell Script

You can execute scripts you've written (that are in your present working directory) by typing:

```
./scriptname.sh
```

This tells the server the path to the command it's executing

But we execute other commands by typing just `ls` or `cd` or `echo`

Why can't we just execute the file by typing it's name?

Lesson 2.2:
Executing a Shell Script

Security.

What happens if somebody comes into your directory and creates an executable file called `ls` that contains:

```
#!/bin/bash
echo "sucks to be you"
rm -rf /
```

(Don't create this file or run `rm -rf /`)

Lesson 2.2:
Executing a Shell Script

Security.

What happens if somebody comes into your directory and creates an executable file called `ls` that contains:

```
#! /bin/bash
echo “sucks to be you”
rm –rf /
```

This way, you can be sure that you’re using the genuine `ls` command.

Lesson 2.2:
Executing a Shell Script

So how do we execute `hello.sh`?

Lesson 2.2:
Executing a Shell Script

So how do we execute `hello.sh`?

```
./hello.sh
```

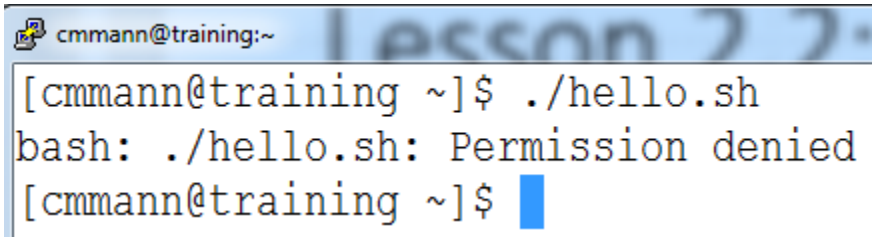
What happens when you run the script?

Lesson 2.2:
Executing a Shell Script

So how do we execute `hello.sh`?

```
./hello.sh
```

What happens when you run the script?

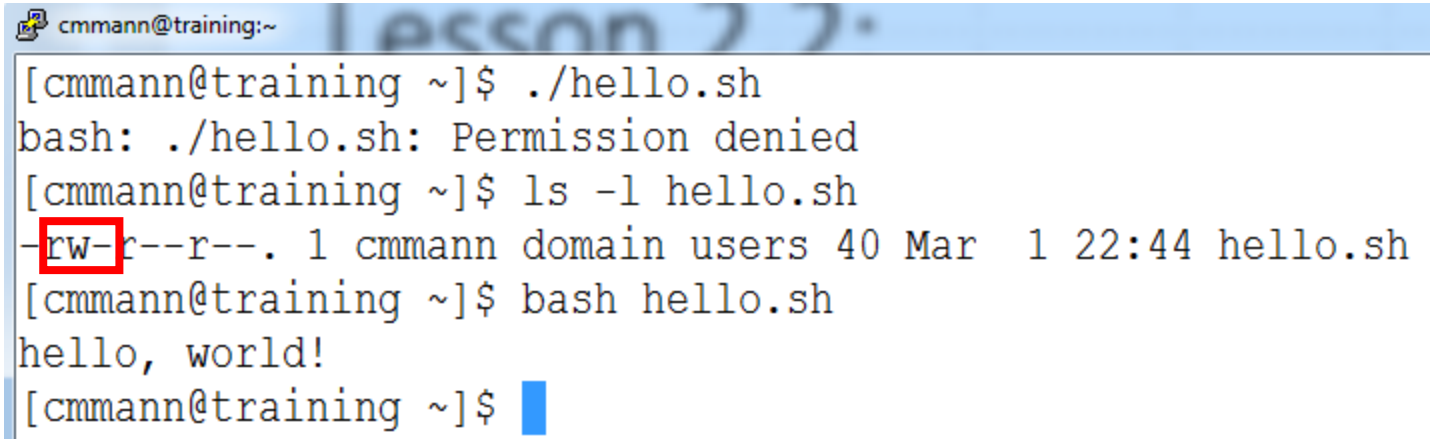


Lesson 2.2:
Executing a Shell Script

See what happens with:

```
bash hello.sh
```

Lesson 2.2:
Executing a Shell Script



Why is the script executing, even though we don't have permission!?!?

Lesson 2.3: Executing a Shell Script

Fun fact: The execute permission is not a *security* feature – instead, it's a flag to the system that a script is executable, and the system now knows to look for a `#!` header line to know what program to use to *interpret* the instructions in your script.

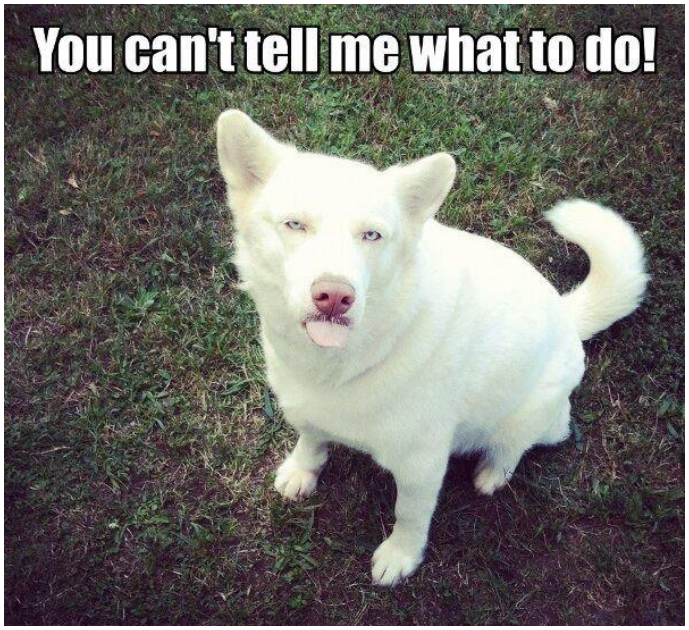
So when we run a script with `./hello.sh`, we are executing *hello.sh*, which the system does not recognize as executable, and so it does not use bash to execute it

When we run the script with `bash hello.sh`, we are executing *bash*, which is reading `hello.sh` and then executing the commands it has read

Lesson 2.3: Executing a Shell Script

The difference between the two:

In scenario 1, `hello.sh` is telling the system what to do, but the system hasn't been told how to understand those instructions



In scenario 2, `bash` is reading `hello.sh`, and then `bash` is telling the system what to do

`bash` has executable permissions, so it can 'boss' the system around, but `hello.sh` currently doesn't, so it can't

Lesson 2.3:
Executing a Shell Script

Try changing the permissions on `hello.sh` to make it executable for you, the owner

How would you change the Execute permission for hello.sh?

```
chmod ??? hello.sh
```

Remember: read = 4, write = 2, execute = 1

Lesson 2.3:
Executing a Shell Script

Exercise 2:

Try changing the permissions on hello.sh to make it executable for you, the owner

How would you change the execute permission for hello.sh?

```
chmod ??? hello.sh
```

Remember: read = 4, write = 2, execute = 1

```
chmod 755 hello.sh
```

Alternate shortcut:

```
chmod u+x hello.sh
```

Lesson 2.3:
Executing a Shell Script

Try executing the script now:

`./hello.sh`

Lesson 2.3:
Executing a Shell Script

If Execute permission isn’t providing security, then what is?

Lesson 2.3:
Executing a Shell Script

If Execute permission isn't providing security, then what is?

Read and Write permissions!

Try changing permission of `hello.sh` so that you have Write and Execute, but not Read:

Lesson 2.3:
Executing a Shell Script

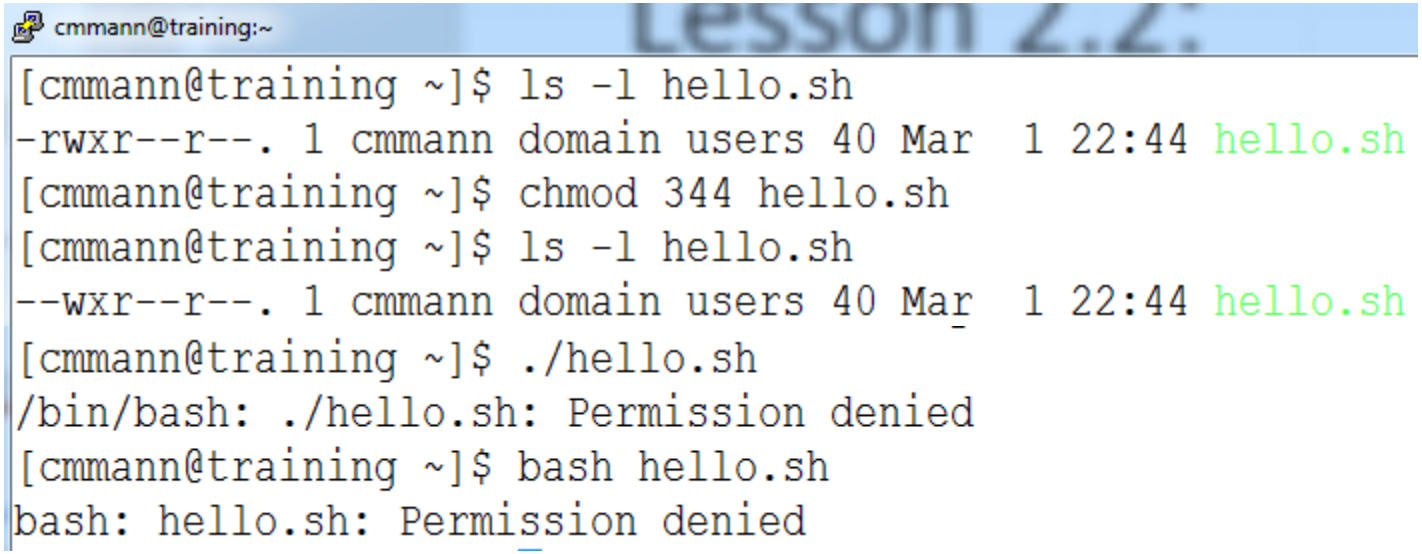
If Execute permission isn't providing security, then what is?

Read and Write permissions!

Try changing permission of `hello.sh` so that you have Write and Execute, but not Read:

```
chmod 344 hello.sh
chmod o-x hello.sh
```

Lesson 2.3:
Executing a Shell Script



Lesson 2.3:
Executing a Shell Script

Why don’t they work?

Lesson 2.3:
Executing a Shell Script

Why don't they work?

Because without Read permission, the system can't read the commands in the file, regardless of how it's called!

So Read (and to a lesser extent, Write) permissions are the true 'security' features of permissions

(if the owner of the shell script file doesn't have Write permissions where the script is operating, the script can't make any changes to the system)

Exercise 2:

Goal:

1. Execute `hello.sh` by calling

```
./hello.sh
```

Lesson 3: Loops and Arguments

Lesson 3.1: Loops

Lesson 3.2: Loop Syntax

Lesson 3.3: Arguments

Lesson 3.4: Passing arguments to a script

Lesson 3.1: Loops

Frequently, we want to do the same action over and over and over again, but to different things

Examples?

Lesson 3.1: Loops

Inefficient way to do this:

```
./Trimmomatic file1.fastq
./Trimmomatic file2.fastq
./Trimmomatic file3.fastq
./Trimmomatic file4.fastq
                        .
                        .
                        .
./Trimmomatic file5.fastq
```

Lesson 3.1: Loops

Efficient way to do this:

```
./trim_loop.sh .
```

```
#! /bin/bash
for file in $1/*
do
     ./Trimmomatic $file
done;
```

Lesson 3.2: Loop Syntax

```
#! /bin/bash

for <variable> in <set>
do
     <something>
done;
```

Lesson 3.2: Loop Syntax

The <variable> in a loop can be anything, as can the <set>

```
for n in 1 2 3 4 5
```

Will loop through the numbers 1, 2, 3, 4, 5

Lesson 3.2: Loop Syntax

We can also loop through files in a directory:

```
for file in /home/cmmann/*
```

(The /* is required to make this run through the directory)

Lesson 3.2: Loop Syntax

We access the <variable> in the set using a dollar sign:

```
for n in 1 2 3 4 5
do
     echo $n
done;
```

Lesson 3.3: Arguments

Not that kind of argument

Lesson 3.3: Arguments

Arguments are parameters that control how a script behaves

Command-line arguments are arguments that you pass through the command line to a script

Arguments can be file names, options, directories, etc.

Lesson 3.3: Arguments

You can access the arguments from the command line in your file using dollar signs and numbers

```
./script.sh arg1 arg2 arg3 arg4
```

```
$1 $2 $3 $4
```

Exercise 3:

1. Navigate to exercise3
2. Open exercise3.sh
3. Follow the directions
4. Check your answers in exercise3answers.sh

Lesson 4:

Overview:

Lesson 4.0: Review Text Output

Lesson 4.1: Word Count

Lesson 4.2: Piping, overwriting, and appending

Lesson 4.3: Sort

Lesson 4.4: Uniq

Lesson 4.5: Grep

Exercise 4: Hello

Lesson 4.0: Text Output

Commands:

`cat <filename.txt>`

`head <filename.txt>`

`tail <filename.txt>`

`less <filename.txt>`

What they do:

`cat` outputs the entirety of `<filename.txt>` to the console (don't try this with large files!!)

`head` outputs the first 10 lines of the file

`tail` outputs the last 10 lines of the file

`less` lets you scroll around a file

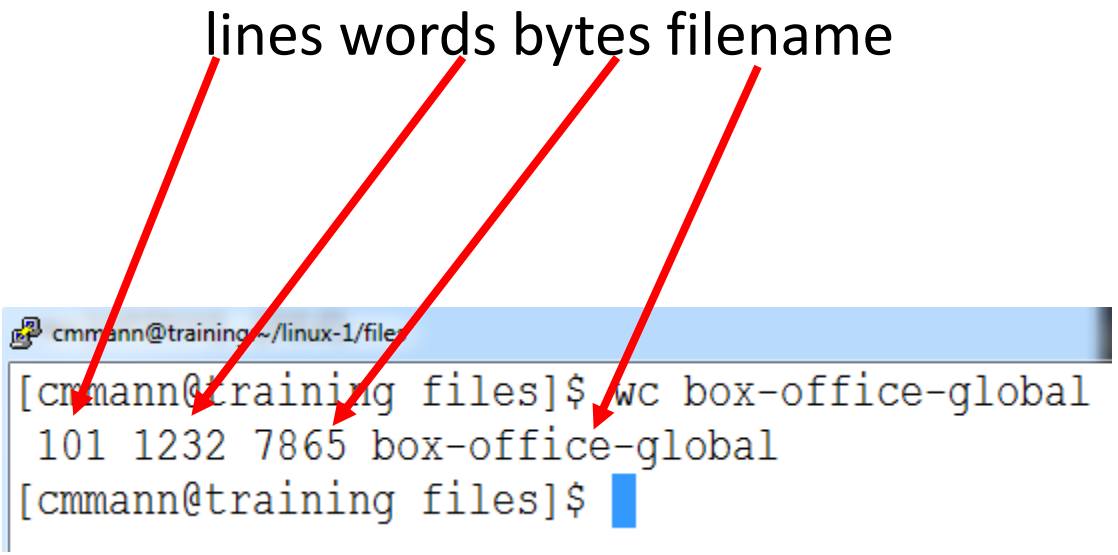
Lesson 4.1: Word Count

Command:

`wc <filename>`

What it does:

Outputs the number of:



Lesson 4.1: Word Count

Options:

`-l` : output ONLY the number of LINES and filename

`-w` : output ONLY the number of WORDS and filename

`-m` : print the number of characters in the file and filename

Lesson 4.1: Word Count

So that's cool, but these options all put out the filename as well

How do we get around that?

Many, many possible ways, but we're going to use piping for now

Lesson 4.2: Piping

We can take the output of one command, and directly feed it to another command – all in one line, using the **[|]** key (this is generally directly below the backspace key)

```
command1 | command2
```

Example:

```
[cmmann@training files]$ wc bill-of-rights
  10  482 2797 bill-of-rights
[cmmann@training files]$ cat bill-of-rights | wc -l
10
```

Lesson 4.3: sort

Command:

`sort <file>`

What it does:

Sorts `<file>` alphabetically by line

Options:

`-n` : sort numerically (if there are no numbers, it will default to alphabetic sort

`-r` : sort in reverse alphabetical order

`-u` : sort only unique items

Lesson 4.4: uniq

Command:
`uniq`

What it does:
Finds unique occurrences of text input

Options:
`-c` : count the occurrences of each line
`-d` : print only duplicated lines
`-u` : print only unique lines

Lesson 4.4: uniq

`uniq` must be called on something that is already sorted!

It works by comparing adjacent items in a list and discarding if they are identical.

Generally called after sort:

```
cat hello.txt | sort | uniq
```

Lesson 4.5: Grep

Stands for “Global Regular Expression Print”

EXTREMELY POWERFUL search tool

Finds text matching highly variable criteria and prints the lines containing that text

Can search multiple files, and find the files that match

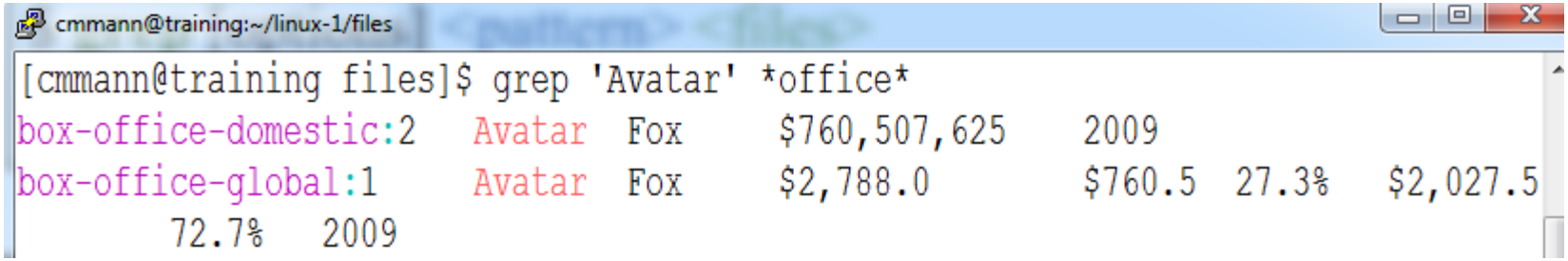
Lesson 4.5: Grep

Command:

`grep -options <pattern> <files>`

What it does:

`grep` searches `<files>` for content matching `<pattern>`



Lesson 4.6: Piping and Grep

We can also feed text directly to grep, and have it search that:

Command:

`<intext> | grep –options <pattern>`

What it does:

grep searches `<intext>` for content matching `<pattern>`

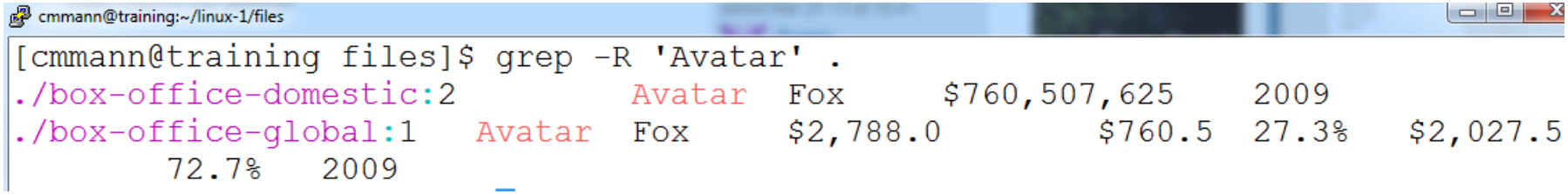
```
[cmmann@training files]$ cat box-office-global | grep 'Avatar'
1       Avatar  Fox     $2,788.0        $760.5  27.3%   $2,027.5        72.7%
009
```

Lesson 4.7:
Grep All Files in A Directory

We can also search for content within a directory:

```
grep –R <pattern> <directoryname/>
```

For this, we have to use the –R Recursive option!



Lesson 4.8: Grep Options

Grep has many, many options:

`-c` : count how many LINES on which the pattern occurs

`-o` : show only the part of a line that matches a pattern; this will show all matches in the line

`-v` : invert match – so select things that DON'T match `<pattern>`

`-i` : case insensitive matching

`-l` : list the files with a match

`-L` : list the files that don't have a match

Exercise 4: Hello

1. Navigate to `~/20181013-adv-unix/exercise4/`
2. Open "`exercise4.sh`"
3. Edit the file to perform the exercises.
4. Execute the file!

Hint:

If you aren't sure if you're getting the correct answers, you can run `exercise4answers.sh`.

Lesson 5: Regular Expressions

Overview:

Lesson 5.1: What are Regular Expressions?

Lesson 5.2: `egrep`

Lesson 5.3: Matching words with `egrep`

Lesson 5.4: Fuzzy Matching

Lesson 5.5: Number Matching

Lesson 5.6: Operators

Lesson 5.7: Matching X Letters

Lesson 5.8: Example

Lesson 5.9: Continuing Education

Lesson 5.1: Regular Expressions

Also called ‘regex’ or ‘regexp’

UNBELIEVABLY POWERFUL tool for defining search patterns

Consists of ‘codes’ that denote various conditions

These conditions can be used to very narrowly find things, or very, very broadly find things

Lesson 5.2: Regular Expressions

In UNIX, frequently used with `grep`

```
grep -E <'regexppattern'> <file>
```

The option "`-E`" tells grep that the pattern is a regular expression!

It is very important that you remember the "-E" option, otherwise grep will try to match your exact pattern, instead of what it represents.

Lesson 5.2: egrep

Alternatively, you can use egrep:

```
egrep <'regexppattern'> <file>
```

This behaves exactly as "`grep -E`", and will be used through the rest of the slides.

Lesson 5.3: Matching Words

We can still match words while grepping regular expressions:

```
egrep 'cat' <file>
```

will still find any instance of the letters ‘cat’ in a file

But grep allows us to search for words
similar to ‘cat’…

Lesson 5.4: Fuzzy Matching

The regexp to find words containing ‘cat’ or ‘cot’ would be:

‘[c][ao][t]’

The brackets encase ‘character’ slots

What would ‘[fw][i][s][h]’ match?

Lesson 5.4: Fuzzy Matching

The regexp to find words containing ‘cat’ or ‘cot’ would be:

‘[c][ao][t]’

The brackets encase ‘character’ slots

What would ‘[fw][i][s][h]’ match?

fish, lungfish, fishing, wish, wishing, swish, etc.

Lesson 5.4: Fuzzy Matching

If we only wanted to match the ‘word’ cat or cot, and not , we can bracket ‘[c][ao][t]’ with spaces:

‘[ ][c][ao][t][ ]’

Note that many, many systems use Regular Expressions, and some have slightly different usage.

For many systems, you can specify a match to ‘whitespace’ (spaces and tabs) using “\s”, but this does not work in bash.

Lesson 5.4: Fuzzy Matching

This bracket system, though, is rather cumbersome. Instead, we could specify:

‘\b[c][ao][t]’

In this context, ‘\b’ means to match the beginning of a word.

The ‘\’ before the ‘b’ is an *escape* character – it signals that we don’t want to *literally* match the letter ‘b’, but the condition that ‘b’ represents.

Lesson 5.4: Fuzzy Matching

We can use a ‘-’ to represent a span of characters:

‘[a-c][o][g]’ would recognize ‘aog’, ‘bog’, ‘cog’

‘[l-z][o][g]’ would only recognize ‘log’, ‘mog’, ‘nog’ etc.

Lesson 5.5: Number Matching

We can also match numbers:

What number(s) will the following match?

‘[0-3][5-8][345]’

Lesson 5.5: Number Matching

We can also match numbers:

What number(s) will the following match?

‘[0-3][5-8][345]’

053, 153, 374, etc.

Lesson 5.6: Operators

‘[cd][ao][tg]’ would match ‘cat’ or ‘dog’

(But also ‘cag’, ‘dat’, and any combination of those letters)

What regular expression would you use to find words containing “trap” or “tarp”?

Lesson 5.6: Operators

‘[cd][ao][tg]’ would match ‘cat’ or ‘dog’

(But also ‘cag’, ‘dat’, and any combination of those letters)

What regular expression would you use to find words containing “trap” or “tarp”?

‘[t][ar][ar][p]’

Lesson 5.6: Operators

But what if we wanted to match ‘trap’ or ‘tarp’, but not ‘trrp’ or ‘taap’?

We can use *operators* to specify this!

Lesson 5.6: Operators

If you want to match *this* OR *that*:

```
egrep 'this|that' <file>
```

When using regular expressions, grep understands that "|" means "OR"

If you to find things that are NOT something, you use:

```
egrep –v 'something' <file>
```

Lesson 5.6: Operators

What if you want to match the character ‘|’?

We use escape characters again!

```
egrep '\|'
```

Lesson 5.7:
Matching X Letters

What if we want to find something more complicated, like a zip code?

What is the form of a zip code?

5 numbers

How could we potentially match that?

‘[0-9][0-9][0-9][0-9][0-9]’

Lesson 5.7:
Matching X Letters

But that's rather cumbersome. Instead, we can specify a specific number of times to look for a set of characters:

```
egrep '[0-9]{5}' <file>
```

In regexp, you can use a number in brackets AFTER the thing that you want to repeat

Lesson 5.7:
Matching X Letters

We can put more than just a number in there:

`a{n,}` : will match the letter ‘a’ `n` OR MORE times

What will ‘`a{2,}`’ match?

aardvark, armadillo, aaaah

Lesson 5.7:
Matching X Letters

We can put more than just a number in there:

`a{n,}` : will match the letter ‘a’ `n` OR MORE times

What will ‘`a{2,}`’ match?

aardvark, armadillo, aaaah

Lesson 5.7: Matching X Letters

We can also specify a range of times to match:

`a{n, m}` : will match ‘a’ at least `n` times, but not more than `m` times.

What will ‘`a{2, 3}`’ match?

aardvark, armadillo, aaaah

Lesson 5.7:
Matching X Letters

We can also specify a range of times to match:

`a{n, m}` : will match ‘a’ at least `n` times, but not more than `m` times.

What will ‘`a{2, 3}`’ match?

aardvark, armadillo, aaaah

Lesson 5.7: Matching X Letters

We can also specify more matches:

`a*` : match ‘a’ 0 or more times

`a+` : match ‘a’ 1 or more times

`a?` : match ‘a’ once if it happens, but matching it is optional

Lesson 5.8: Example

We can match EXTREMELY complicated things

Real world example: PDB files

In my day job, I want to find the coordinates of atoms in PDB files.

These lines take the form:

```
ATOM      1  N   SER A  44       0.312  28.338  23.824  1.00109.80           N
ATOM      2  CA  SER A  44      -1.014  28.655  23.237  1.00113.84           C
ATOM      3  C   SER A  44      -1.893  27.385  23.044  1.00115.10           C
ATOM      4  O   SER A  44      -1.573  26.307  23.566  1.00111.94           O
```

```
ATOM   1589  O3'   A B   9       4.770  39.279  56.136  1.00228.34           O
ATOM   1590  C2'   A B   9       2.693  40.521  56.600  1.00214.10           C
ATOM   1591  O2'   A B   9       3.406  41.227  57.593  1.00219.27           O
ATOM   1592  C1'   A B   9       1.906  41.493  55.715  1.00207.15           C
```

Lesson 5.8: Example

So these lines look similarly, but they have different numbers and characters spaced differently.

And the rest of the file looks NOTHING like this.

How could I pull out ONLY these lines?

```
ATOM      1  N   SER A  44       0.312  28.338  23.824  1.00109.80           N
ATOM      2  CA  SER A  44      -1.014  28.655  23.237  1.00113.84           C
ATOM      3  C   SER A  44      -1.893  27.385  23.044  1.00115.10           C
ATOM      4  O   SER A  44      -1.573  26.307  23.566  1.00111.94           O
```

```
ATOM   1589  O3'   A B   9       4.770  39.279  56.136  1.00228.34           O
ATOM   1590  C2'   A B   9       2.693  40.521  56.600  1.00214.10           C
ATOM   1591  O2'   A B   9       3.406  41.227  57.593  1.00219.27           O
ATOM   1592  C1'   A B   9       1.906  41.493  55.715  1.00207.15           C
```

Lesson 5.8: Example

We could try:

`egrep 'ATOM' 1R2X.pdb`, but…

```
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
```

```
ATOM      1  N   SER A  44       0.312  28.338  23.824  1.00109.80           N
ATOM      2  CA  SER A  44      -1.014  28.655  23.237  1.00113.84           C
ATOM      3  C   SER A  44      -1.893  27.385  23.044  1.00115.10           C
ATOM      4  O   SER A  44      -1.573  26.307  23.566  1.00111.94           O
```

```
ATOM   1589  O3'   A B   9       4.770  39.279  56.136  1.00228.34           O
ATOM   1590  C2'   A B   9       2.693  40.521  56.600  1.00214.10           C
ATOM   1591  O2'   A B   9       3.406  41.227  57.593  1.00219.27           O
ATOM   1592  C1'   A B   9       1.906  41.493  55.715  1.00207.15           C
```

Lesson 5.8: Example

We can specify that we only want to match ‘ATOM’ if it starts at the beginning of the line:

```
egrep '^ATOM' 1R2X.pdb
```

The character ‘^’ is a special character called an ‘anchor’ that means to match the beginning of the line

Lesson 5.8: Example

But what if I ONLY want the protein atom coordinates?

```
ATOM      1  N   SER A  44       0.312  28.338  23.824  1.00109.80           N
ATOM      2  CA  SER A  44      -1.014  28.655  23.237  1.00113.84           C
ATOM      3  C   SER A  44      -1.893  27.385  23.044  1.00115.10           C
ATOM      4  O   SER A  44      -1.573  26.307  23.566  1.00111.94           O
```

```
ATOM   1589  O3'   A B   9       4.770  39.279  56.136  1.00228.34           O
ATOM   1590  C2'   A B   9       2.693  40.521  56.600  1.00214.10           C
ATOM   1591  O2'   A B   9       3.406  41.227  57.593  1.00219.27           O
ATOM   1592  C1'   A B   9       1.906  41.493  55.715  1.00207.15           C
```

Lesson 5.8: Example

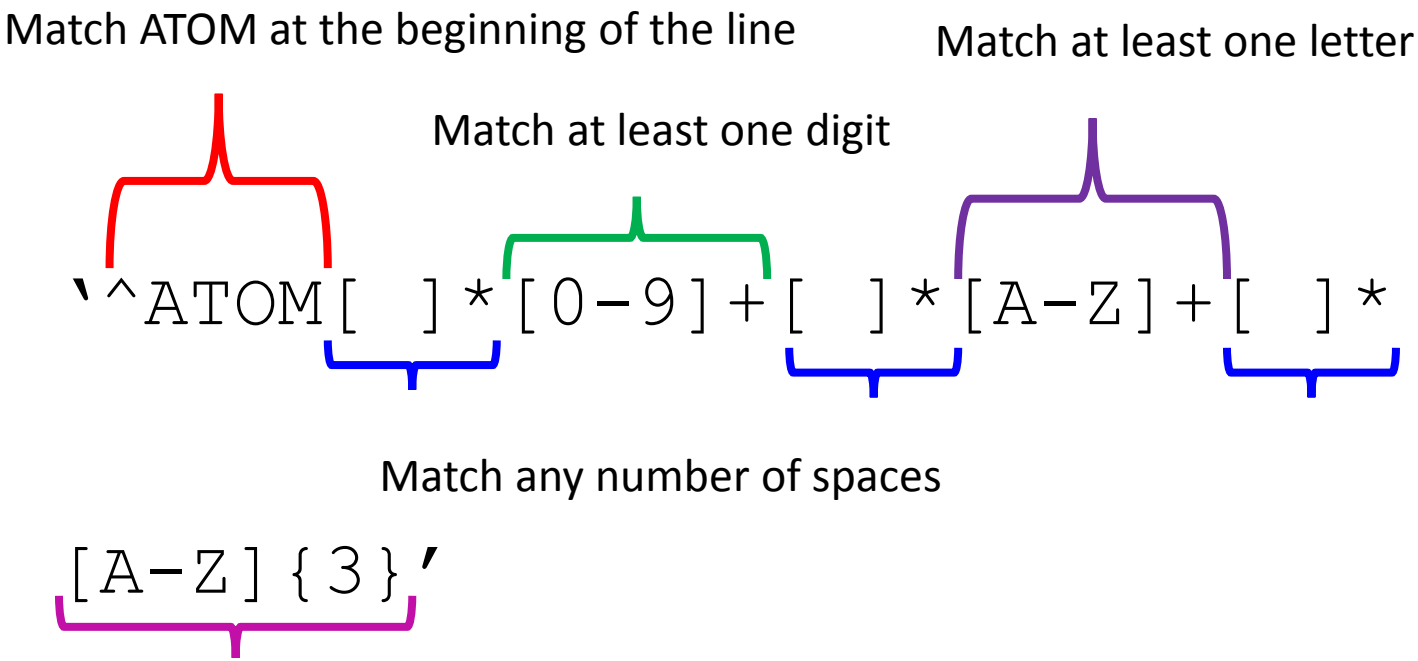
We make a really *complicated* regexp:

```
egrep '^ATOM[ ]*[0-9]+[ ]*[A-Z]+[
]*[A-Z]{3}'
```

```
ATOM      1  N   SER A  44       0.312  28.338  23.824  1.00109.80           N
ATOM      2  CA  SER A  44      -1.014  28.655  23.237  1.00113.84           C
ATOM      3  C   SER A  44      -1.893  27.385  23.044  1.00115.10           C
ATOM      4  O   SER A  44      -1.573  26.307  23.566  1.00111.94           O
```

Lesson 5.8: Example

What is this doing?



Lesson 5.9:
Regexp Continuing Education

There are many, many more options available to use with regexp in bash

We could spend an entire workshop on this alone. (We're not going to today, though.)

If you want to learn more, visit:

http://tldp.org/LDP/Bash-Beginners-Guide/html/sect_04_01.html#sect_04_01_02

Exercise 5: Real Life Stuff

1. Open and edit `exercise5.sh`
2. Complete the exercises within.
3. Run `exercise5.sh`

Closing

Thanks for coming!

Please take this survey so that we can improve the workshop for future attendees:

https://goo.gl/forms/cumiG8DvCOzOmDuC2