

Simple Shell Scripting for Scientists

Day Two

Anna Langley
Ben Harris
University of Cambridge Information Services

Introduction

- Who:
 - Anna Langley, Infrastructure Division, UIS
 - Ben Harris, Infrastructure Division, UIS
- · What:
 - Simple Shell Scripting for Scientists course, Day One
 - Part of the Scientific Computing series of courses
- Contact (questions, etc):
 - scientific-computing@uis.cam.ac.uk
- Health & Safety, etc:
 - Fire exits
- · Please use mobiles considerately

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

As this course is part of the Scientific Computing series of courses run by the University Information Services, all the examples that we use will be more relevant to scientific computing than to system administration, etc.

This does not mean that people who wish to learn shell scripting for system administration and other such tasks will get nothing from this course, as the techniques and underlying knowledge taught are applicable to shell scripts written for almost any purpose. However, such individuals should be aware that this course was not designed with them in mind.

Version: Lent 2020 1 Version: Lent 2020 2

We finish at:

17:00

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

The course officially finishes at 17.00, so don't expect to finish before then. If you need to leave before 17.00 vou are free to do so, but don't expect us to have covered all today's material by then. How quickly we get through the material varies depending on the composition of the class, so whilst we may finish early you should not assume that we will. If you do have to leave early, please leave quietly.

If, and only if, you will not be attending the next day of the course then please make sure that you fill in the Course Review form online, accessible under "feedback" on the main MCS Linux menu, or via:

http://feedback.training.cam.ac.uk/uis/

What we don't cover

- Different types of shell:
 - We are using the Bourne-Again SHell (bash).
- Differences between versions of bash.
- Very advanced shell scripting try one of these courses instead:
 - "Python 3: Introduction for Absolute Beginners"
 - "Python 3: Introduction for Those with Programming Experience"

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

bash is the most common shell on modern Unix/Linux systems – in fact, on most modern Linux distributions it will be the default shell (the shell users get if they don't specify a different one). Its home page on the WWW is at:

https://www.gnu.org/software/bash/

We will be using bash 4.4 in this course, but everything we do should work in bash 2.05 and later. Version 4, version 3 and version 2.05 (or 2.05a or 2.05b) are the versions of bash in most widespread use at present. Most recent Linux distributions will have one of these versions of bash as one of their standard packages. The latest version of bash (at the time of writing) is bash 5.0, which was released in January 2019.

For details of the "Python 3: Introduction for Absolute Beginners" course, see:

https://www.training.cam.ac.uk/ucs/course/ucs-python For details of the "Python 3: Introduction for Those with Programming" Experience" course, see:

https://www.training.cam.ac.uk/ucs/course/ucs-python4progs Version: Lent 2020

Outline of Course

- 1. Recap of day one
- 2. Shell functions

SHORT BREAK

- Command substitution
- 4. The **mktemp** command

VERY SHORT BREAK

- Handling data from standard input
 - Reading values from standard input
 - Pipelines
 - Loop constructs: while

SHORT BREAK

- More while loops:
 - Shell arithmetic
 - Tests

Exercise

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

The course officially finishes at 17.00, but the intention is that the lectured part of the course will be finished by about 16.30 or soon after, and the remaining time is for you to attempt an exercise that will be provided. If you need to leave before 17.00 (or even before 16.30), please do so, but don't expect the course to have finished before then. If you do have to leave early, please leave quietly.

If, and only if, you will not be attending the next day of the course then please make sure that you fill in the Course Review form online, accessible under "feedback" on the main MCS Linux menu, or via:

http://feedback.training.cam.ac.uk/uis/



As this is a shell scripting course, we are going to need to interact with the Unix shell.

To start a shell, click on "Activities" in the top-left corner of the screen, then click on the "Terminal" icon in the desktop application bar.

A Terminal window will then appear.

 version: Lent 2020
 5
 Version: Lent 2020
 6

Recap: Day One

- Simple shell scripts: linear lists of commands
- Simple use of shell variables and parameters
- Simple command line processing
- Output redirection
- for loops

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

Recap: What is a shell script?

- Text file containing commands understood by the shell
- Very first line is special:
 #!/bin/bash
- File has its executable bit set chmod a+x

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

Recall that the **chmod** command changes the permissions on a file. **chmod a+x** sets the executable bit on a file for all users on the system, i.e. it grants everyone permission to execute the file. (*Note* though, that all files in your home directory on the MCS Linux systems used in this course automatically have their executable bit set, so during this course you don't need to explicitly use the **chmod** command on such files.) Unix file permissions were covered in the "Unix: Introduction to the Command Line Interface" course, see:

https://www.training.cam.ac.uk/ucs/course/ucs-unixintro1

The notes from this course are available on-line at:

https://help.uis.cam.ac.uk/help-support/training/downloads/course-files/programming-student-files/unix-cli

Version: Lent 2020 7 Version: Lent 2020 8

Recap: Very simple shell scripts

- Linear lists of commands
- Just the commands you'd type interactively put into a file
- · Simplest shell scripts you'll write

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

Shell variables and parameters

Shell variables hold data, much like variables in a program:

```
$ var="My variable"
$ echo "${var}"
My variable
```

Shell parameters are special variables set by the shell:

- Positional parameter 0 holds the name of the shell script
- Positional parameter 1 holds the first argument passed to the script; positional parameter 2 holds the second argument passed to the script, etc
- Special parameter @ expands to values of all positional parameters (starting from 1)
- Special parameter # expands to the number of positional parameters (not including 0)

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

10

We create shell variables by simply assigning them a value (as above for the shell variable VAR). We can access a the value of a shell variable using the construct **SVARIABLE** where **VARIABLE** is the name of the shell variable. Note that there are **no** spaces between the name of the variable, the equal sign (=) and the variable's value in double quotes. **This** is very important as whitespace (spaces, tabs, etc) is significant in the names and values of shell variables.

Also note that although we can assign the value of one shell variable to another shell variable, e.g. VAR1=\$ {VAR}, the two shell variables are in fact completely separate from each other, i.e. each shell variable can be changed independently of the other. Changing the value of one will not affect the other. So VAR1 (in this example) is not a "pointer" to or an "alias" for VAR.

Shell parameters are special variables set by the shell. Many of them cannot be modified, or cannot be directly modified, by the user or by a shell script. Amongst the most important parameters are the positional parameters and the other shell parameters associated with them.

The positional parameters are set to the arguments that were given to the shell script when it was started, with the exception of positional parameter 0, which is set to the name of the shell script. So, if myscript is a shell script, and I ran it by typing:

./myscript argon hydrogen mercury

then positional parameter

 $\mathbf{0} = ./\mathrm{myscript}$

1 = argon

2 = hydrogen

3 = mercury

and all the other positional parameters are not set.

The special parameter @ is set to the value of all the positional parameters, starting from the first parameter, passed to the shell script, each value being separated from the previous one by a space. You access the value of this parameter using the construct \${@}. If you access it in double quotes – as in "\${@}" – then the shell will treat each of the positional parameters as a separate word (which is what you normally want).

The special parameter # is set to the number of positional parameters not counting positional parameter 0. Thus it is set to the number of arguments passed to the shell script, i.e. the number of arguments on the command line when the shell script was run.

Version: Lent 2020 9 Version: Lent 2020 10

Shell parameters

- Positional parameters (\$0, \$1, etc)
- Value of all arguments passed: \$@
- Number of arguments: \$#

\$ cd

\$ examples/params 0.5 62 38 hydrogen

This script is /home/y250/examples/params

There are 4 command line arguments.

The first command line argument is: 0.5 The second command line argument is: 62 The third command line argument is: 38

Command line passed to this script: 0.5 62 38 hydrogen

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

In the examples subdirectory of your home directory there is a script called **params**. If you run this script with some command line arguments it will illustrate how the positional parameters and related shell parameters work. Note that even if you type exactly the command line on the slide above your output will probably be different as the script will be in a different place for each user.

The positional parameter **0** is the name of the shell script (it is the name of the command that was given to execute the shell script).

The positional parameter **1** contains the first argument passed to the shell script, the positional parameter **2** contains the second argument passed and so on.

The special parameter # contains the number of arguments that have been passed to the shell script. The special parameter @ contains all the arguments that have been passed to the shell script.

for

Execute some commands once for each value in a collection of values

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

12

We can repeat a set of commands using a **for** loop. A **for** loop repeats a set of commands once for each value in a collection of values it has been given. We use a **for** loop like this:

```
for VARIABLE in <collection of values> ; do
    <some commands>
```

done

where <collection of values> is a set of one or more values (strings of characters). Each time the for loop is executed the shell variable VARIABLE is set to the next value in <collection of values>. The two most common ways of specifying this set of values is by putting them in a another shell variable and then using the \${} construct to get its value (note that this should not be in quotation marks), or by using a wildcard or file name glob (e.g. *) to specify a collection of file names (pathname expansion). <some commands> is a list of one or more commands to be executed.

Note that you can put the ${\bf do}$ on a separate line, in which case you can omit the semi-colon (;):

There are some examples of how to use it in the **for1** and **for2** scripts in the examples directory of your home directory. Note that a **for** loop can contain another **for** loop (the technical term for this is *nestinq*).

version: Lent 2020 11 version: Lent 2020 12

Recap: What are we trying to do? Scientific computing i.e. shell scripts that do some useful scientific work, e.g. repeatedly running a simulation or analysis with different data scientific-computing@uis.cam.ac.uk Simple Shell Scripting for Scientists: Day Two 13

Recall the name of this course ("Simple Shell Scripting for Scientists") and its purpose: to teach you, the scientist, how to write shell scripts that will be useful for your *scientific work*.

As mentioned on the previous day of the course, one of the most common (and best) uses of shell scripts is for automating repetitive tasks. Apart from the sheer tediousness of typing the same commands over and over again, this is exactly the sort of thing that human beings aren't very good at: the very fact that the task is repetitive increases the likelihood we'll make a mistake (and not even notice at the time). So it's much better to write (once) – and test – a shell script to do it for us. Doing it via a shell script also makes it easy to *reproduce* and *record* what we've done, two very important aspects of any scientific endeavour.

So, the aim of this course is to equip you with the knowledge and skill you need to write shell scripts that will let you run some program (e.g. a simulation or data analysis program) over and over again with different input data and organise the output sensibly.

Sample program: **zombie** (1)

6 ./zombie 0.005 0.0175 0.01 0.01 500

```
When Zombies Attack!: Basic Model of outbreak of zombie infection
Population size:
                        5.0000e+05
Model run time:
                        1.0e+01 days
Zombie destruction rate (alpha):
                                         5.000000e-03
Zombie infection rate (beta):
                                         1.750000e-02
                                         1.000000e-02
Zombie resurrection rate (zeta):
Natural death [and birth] rate (delta): 1.000000e-02
Output file:
                         zombie.dat
Model took 7.457018e-02 seconds
                                   Simple Shell Scripting for Scientists: Day Two
                                                                                          14
```

The **zombie** program is in your home directory. It is a program written specially for this course, but we'll be using it as an example program for pretty general tasks you might want to do with many different programs. Think of **zombie** as just some program that takes some input on the command line and then produces some output (on the screen, or in one or more files, or both), e.g. a scientific simulation or data analysis program.

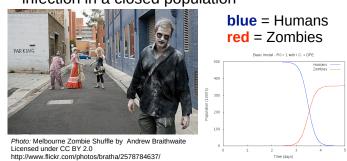
The **zombie** program takes 5 numeric arguments on the command line: 4 positive floating-point numbers and 1 positive integer. It always writes its output to a file called zombie.dat in the current working directory, and also writes some informational messages to the screen.

The **zombie** program is not as well behaved as we might like (which, sadly, is also typical of many programs you will run). The particular way that **zombie** is not well behaved is this: every time it runs it creates a file called running-zombie in the current directory, and it will not run if this file is already there (because it thinks that means it is already running). Unfortunately, it doesn't remove this file when it has finished running, so we have to do it manually if we want to run it multiple times in the same directory.

Version: Lent 2020 13 Version: Lent 2020 14

Sample program: zombie (2)

Simulation of an outbreak of a zombie infection in a closed population



The **zombie** program uses a variant of the SIR model from epidemiology to simulate an outbreak of a zombie infection in a closed (i.e. no one enters or leaves) population. Obviously, since zombies don't actually exist, it would be a mistake to try and take this program too seriously. You should think of **zombie** as just a program that takes some input on the command line and then produces some output on the screen and in a file, and whose output can then be fed to yet other programs for further processing (as we'll see later this afternoon).

Simple Shell Scripting for Scientists: Day Two

scientific-computing@uis.cam.ac.uk

However, as it happens, the program is based on actual academic modelling of the spread of disease, as found in Chapter 4 (pp. 133-150) of Infectious Disease Modelling Research Progress (2009), which is entitled "When Zombies Attack!: Mathematical Modelling of an Outbreak of Zombie Infection", and which you can find here:

http://mysite.science.uottawa.ca/rsmith43/zombies.pdf

And in case you are interested in the book from which that chapter is taken, the ISBN of Disease Modelling Research Progress is 978-1-60741-347-9, it's edited by J. M. Tchuenche & C. Chiyaka and published by Nova Science Publishers, Inc.

Note that the **zombie** program writes its output to a file of numbers rather than producing graphical output. At the end of this afternoon we will see how to produce graphs of its output.

This page intentionally left blank

Deze bladzijde werd met opzet blanco gelaten.

このページは計画的にブランクを残ている

Ta strona jest celowo pusta.

Esta página ha sido expresamente dejada en blanco.

Эта страница нарочно оставлена пустой.

Denne side med vilje efterladt tom.

Ĉi tiu paĝo restas intence vaka.

اين صفحه خالي است

An leathanach seo fágtha folamh in aon turas.

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

This page intentionally left blank: nothing to see here.

version: Lent 2020 15 Version: Lent 2020 16

Exercise from Day One

We have a directory that contains the output of several runs of the **zombie** program in separate files. We have a file of commands that will turn the output into a graph (using **gnuplot**). We want to write a shell script that turns the output from each run into a graph.

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

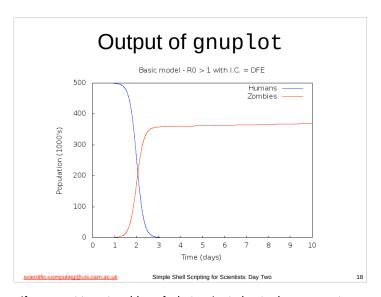
We are specifically using the <code>gnuplot</code> program and the output of the <code>zombie</code> program we met on the previous day of the course. (<code>gnuplot</code> is a program that creates graphs, histograms, etc from numeric data.) Think of this task as basically: I have some data sets and I want to process them all in the same way. My processing might produce graphical output, as here, or it might produce more data in some other format.

If you haven't met **gnuplot** before, you may wish to look at its WWW page:

http://www.gnuplot.info/

If you think you might want to use the **gnuplot** program for creating your own graphs, then you may find the "Introduction to Gnuplot" course of interest – the course notes are on-line at:

https://www-uxsup.csx.cam.ac.uk/courses/moved.Gnuplot/



If you want to get an idea of what we're trying to do, you can try the following:

- \$ cd
- \$ scripts/multi-run 500
- \$ cp gnuplot/zombie.gplt .
- \$ cp zombie-500.dat zombie.dat
- \$ ls zombie.png

/bin/ls: zombie.png: No such file or directory

- \$ gnuplot zombie.gplt
- \$ rm zombie.dat
- \$ ls zombie.png

zombie.png

\$ eog zombie.png &

Note that the output of "**ls zombie.png**" may look slightly different – in particular, the colours may be slightly different shades (assuming you are reading these notes in colour).

version: Lent 2020 17 Version: Lent 2020 18

Details of exercise

What we want to do is, *for* each output file:

- Rename (or copy) the output file we want to process to zombie.dat
- \$ mv zombie-500.dat zombie.dat
- 2. Run gnuplot with the zombie.gplt file
- \$ gnuplot zombie.gplt
- 3. Rename (or delete if you copied the original output file) zombie.dat
- \$ mv zombie.dat zombie-500.dat
- 4. Rename zombie.png
- \$ mv zombie.png zombie-500.dat.png

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

The exercise set at the end of the previous day of the course was to create a shell script that does the above task. Basically, for each of the .dat files produced by the multi-run script, the shell script should run **gnuplot** on it to create a graph (which will be stored as a .png file). The zombie.gplt file provided will only work if the .dat file is called zombie.dat and is in the current directory. Also, **gnuplot** should not be allowed to overwrite each .png file, so the shell script must rename each .png file after **gnuplot** has created it.

multi-gnuplot1

```
File: gnuplot/multi-gnuplot1
#!/bin/bash

# Run gnuplot program once for each output file
for data_file in zombie-*.dat; do

# Rename output file to zombie.dat
mv "$data_file" zombie.dat

# Run gnuplot
gnuplot zombie.gplt

# Rename zombie.dat to original name
mv zombie.dat "$data_file"

# Rename zombie.png
mv zombie.png "$data_file.png"
done
scientific.computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

20
```

So here's one solution to that exercise. This file (multi-gnuplot1) is in the gnuplot directory.

It takes each file whose name is of the form zombie-<something>.dat (where the <something> can be any set of characters that can appear in a filename) in turn and renames it to zombie.dat, runs <code>gnuplot</code>, then renames the file back to its original name, and renames the zombie.png file to zombie-<something>.dat.png.

 Version: Lent 2020
 19
 Version: Lent 2020
 20

multi-gnuplot2

```
File: qnuplot/multi-qnuplot2
   #!/bin/bash
   # Run gnuplot program once for each output file
   for data file in zombie-*.dat; do
     # Copy output file to zombie.dat
     cp -f "$data file" zombie.dat
     # Run anuplot
     gnuplot zombie.gplt
     # Delete zombie.dat file
     rm -f zombie.dat
     # Rename zombie.png
     mv zombie.png "$data_file.png"
   done
scientific-computing@uis.cam.ac.uk
                           Simple Shell Scripting for Scientists: Day Two
                                                                      21
```

 \dots and here's another solution. This file (multi-gnuplot2) is in the gnuplot directory.

It takes each file whose name is of the form zombie-<something>.dat (where the <something> can be any set of characters that can appear in a filename) in turn and copies it to zombie.dat, runs <code>gnuplot</code>, then deletes the copy, and renames the zombie.png file to zombie-<something>.dat.png.

These two shell scripts are functionally equivalent – you can use whichever you like and the results will be identical.

Note that one purely cosmetic difference between them is that one has the **do** keyword on the same line as the **for** keyword (with a semi-colon (;) before the do) whilst the other has the **do** keyword on a separate line (and no semi-colon). Some people feel that it makes scripts more readable to put the **do** on a separate line.

However, whether you put the **do** on the same line as the **for** (and use the semi-colon) or put it on a different line is entirely a matter of style and personal preference – well, you want some outlet for your individuality, don't you? \odot

21

multi-gnuplot3

```
File: gnuplot/multi-gnuplot3
#!/bin/bash

# Run gnuplot program once for each output file
for data_file in zombie-*.dat; do

# Create symbolic link called zombie.dat to output file
ln -s -f "$data_file" zombie.dat

# Run gnuplot
gnuplot zombie.gplt

# Delete zombie.dat symbolic link
rm -f zombie.dat

# Rename zombie.png
mv zombie.png "${data_file}.png"
done
scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two
22
```

 \dots and here's yet another solution. This file (multi-gnuplot3) is also in the gnuplot directory.

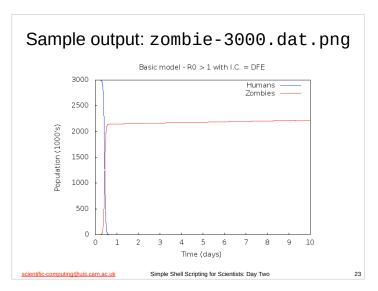
It takes each file whose name is of the form zombie-<something>.dat (where the <something> can be any set of characters that can appear in a filename) in turn and creates a symbolic link to it called zombie.dat, runs gnuplot, then deletes the symbolic link (not the original file), and renames the zombie.png file to zombie-<something>.dat.png.

This shell script is functionally equivalent to the previous two – you can use whichever you like and the results will be identical.

There is, though, one way in which this script is better than the previous two. Since it only creates a symbolic link to each file in turn rather than making a copy of the file (like multi-gnuplot2), it uses considerably less disk space (symbolic links take up almost no space on disk), which can be an issue if the files you are processing are large. Also, since it does not rename the original file (like multi-gnuplot1), if it is interrupted part way through its execution you don't need to worry about potentially "losing" any output files. If multi-gnuplot1 was interrupted after it had renamed a file to zombie. dat but before it had a chance to rename it back, then, unless the person running it realised this had happened and dealt with it, the zombie. dat file would be deleted next time the script was run(!).

22

Version: Lent 2020



You can try out one of these scripts if you want. First, create some output files for the script to process:

\$ cd

\$ rm -f *.dat stdout-* logfile

\$ scripts/multi-run 50 100 500 1000 3000 5000 10000 50000

Now, make sure that the zombie.gplt file is in your current directory: \$ cp gnuplot/zombie.gplt .

Now run one of the scripts, either multi-gnuplot1 or multi-gnuplot2 or multi-gnuplot3, it doesn't matter which:

\$ gnuplot/multi-gnuplot1

Now do an ${f ls}$ to see what files have been created, and then try viewing some of them:

\$ eog zombie-50000.dat.png &

Your solutions to this exercise (you did do it, didn't you?) should have been similar to the ones presented here. If they weren't, or if you had problems with the exercise, please let the course giver or demonstrator know.

Shell functions \$ cd \$ cat hello-function #!/bin/bash function greet() { # This is a shell function. echo "Hello." echo "I am function \${FUNCNAME}." } \$./hello-function

Shell functions are similar to functions in most high-level programming languages. Essentially they are "mini-shell scripts" (or bits of shell scripts) that are invoked (called) by the main shell script to perform one or more tasks. When called they can be passed arguments (parameters), as we will see later, and when they are finished they return control to the statement in the shell script immediately after they were called.

Simple Shell Scripting for Scientists: Day Two

24

To define a function, you just write the following at the start of the function:

```
function function_name()
r
```

scientific-computing@uis.cam.ac.uk

where $\it function_name$ is the name of the function. Then, after the last line of the function you put a line with just a closing curly brace (}) on it:

}

Note that *unlike* function definitions in most high level languages you don't list what parameters (arguments) the function takes. This is not so surprising when you remember that shell functions are like "mini-shell scripts" – you don't explicitly define what arguments a shell script takes either.

Like functions in a high-level programming language, defining a shell function doesn't actually make the shell script do anything – the function has to be called by another part of the shell script before it will actually *do* anything.

FUNCNAME is a special shell variable (introduced in version 2.04 of bash) that the shell sets within a function to the name of that function. When not within a function, the variable is unset.

 Version: Lent 2020
 23
 Version: Lent 2020
 24

Calling a shell function

```
$ gedit hello-function &
#!/bin/bash
function greet()
{
    # This is a shell function.
    echo "Hello."
    echo "I am function $FUNCNAME."
}

greet
$ ./hello-function
Hello.
I am function greet.
$

scientific-computing@uis.cam.ac.uk
Simple Shell Scripting for Scientists: Day Two
25
```

Start your favourite editor (or gedit if you don't have a preference) and modify the file hello-function in your home directory as shown above. *Make sure you save the file after you've modified it or your changes won't take effect.*

Now try running the shell script again:

```
$ ./hello-function
Hello.
I am function hello.
$
```

This time it actually does something – the function ${\tt greet}$ is called and does what we would expect.

You call a shell function by just giving its name (just as you would with any of the standard Unix commands (or shell builtin commands) that we've met). Note that you don't put brackets after the name of the function when you call it. You only do that when you first define the function. That's one of the ways that the shell figures out that you are trying to define a shell function.

Shell function arguments (1)

```
$ gedit hello-function &
#!/bin/bash
function greet()
{
    # This is a shell function.
    echo "Hello, $1"
    echo "I am function $FUNCNAME."
}

greet
$ ./hello-function Dave
Hello,
I am function greet.
$
scientific-computing@uis.cam.ac.uk
Simple Shell Scripting for Scientists: Day Two
```

Modify the file hello-function in your home directory as shown above. Make sure you save the file after you've modified it or your changes won't take effect.

Recall that the positional parameter **1** (whose value is accessed using the construct **\${1}**) contains the value of the first argument passed to the shell script (or is unset if no arguments are passed). So what would we expect the above shell script to do? Surely, it will print out "Hello, <whatever argument we gave it>"?

(For the pedants amongst you: <whatever argument we gave it> means whatever argument we passed the shell script on the command line when we invoked it – "Dave" in the above example.)

Apparently not. Maybe something's wrong with out shell script? Maybe positional parameter **1** isn't being set correctly? Let's try some debugging and see.

Version: Lent 2020 25 Version: Lent 2020 26

Shell function arguments (2)

```
$ gedit hello-function &
#!/bin/bash
function greet()
{
    # This is a shell function.
    echo "Hello, $1"
    echo "I am function $FUNCNAME."
}

echo "First argument: $1"
hello
$ ./hello-function Dave
First argument: Dave
Hello,
I am function greet.
```

Modify the file hello-function in your home directory as shown above. Make sure you save the file after you've modified it or your changes won't take effect.

This is a simple but useful debugging trick for shell scripts. When something isn't working right, make the shell script print out the values of all the shell variables, environment variables or shell parameters that you are interested in *just before* the point where you think it is going wrong.

In this case, what this shows us is that positional parameter ${\bf 1}$ is being set correctly. So that's not the problem.

The problem is that within a function the positional parameters (from $\bf 1$ onward, $\bf 0$ doesn't change) are set to the arguments that the function was given when it was called. (Similarly, within a function the special parameters $\bf 0$ and $\bf 4$ are set to all the arguments passed to the function, and the number of arguments passed to the function, respectively.) Since we called the function $\bf hello$ without any arguments, while the function $\bf greet$ is executing positional parameter $\bf 1$ is unset, and so when we try to print its value, nothing is printed.

The way you call a shell function with arguments is to list those arguments immediately after the name of the shell function, e.g. in our script:

hello Dave

would call the function **greet** with one argument: "Dave".

Shell function arguments (3)

```
$ gedit hello-function &
#!/bin/bash
function greet()
{
    # This is a shell function.
    echo "Hello, $1"
    echo "I am function $FUNCNAME."
}
echo "First argument: $1"
greet Hal
$ ./hello-function Dave
First argument: Dave
Hello, Hal
I am function greet.
```

Modify the file hello-function in your home directory as shown above. Make sure you save the file after you've modified it or your changes won't take effect.

So, if we call our function with an argument (in this case the argument is "Hal"), then the value of the positional parameter **1** is indeed set to that argument within the function.

So, if we want to our function to have the same first argument as the shell script itself, then we need to call the function with the first argument with which the shell script was invoked.

You can probably guess how we do this...

Version: Lent 2020 27 Version: Lent 2020 28

Shell function arguments (4)

```
$ gedit hello-function &
#!/bin/bash
function greet()
{
    # This is a shell function.
    echo "Hello, $1"
    echo "I am function $FUNCNAME."
}

#echo "First argument: $1"
greet "$1"
$ ./hello-function Dave
Hello, Dave
I am function greet.

scientific-computing@uis.cam.ac.uk
Simple Shell Scripting for Scientists: Day Two
```

Modify the file hello-function in your home directory as shown above. Make sure you save the file after you've modified it or your changes won't take effect.

Note that now we think we've cracked it, we can get rid of our debugging effort. We could delete that line, but, if we were wrong, we'd only have to put it back in again as we tried to figure it out. So it is easier to just comment it out by inserting a hash character (#) at the start of the line – recall that the shell treats everything after a hash at the start of a line as a comment.

But as you probably guessed – it does indeed work the way we want. Positional parameter **1** holds the first argument that was given on the command line to the shell script, so if we want to pass that argument to the greet function, we just put:

in our shell script, and voilà!

Why use shell functions?

- Allow us to structure our shell script:
 - Functions ⇔ sub-tasks
- Easier to write small parts of the shell script at a time:
 - So we can write the easy bits first!
- · Easier to test individual parts of the shell script
- Repetitive sequences of commands only appear in one place:
 - Less typing! Fewer typos!
 - Easy to make changes
 - Easy to fix errors
- Can re-use functions in different shell scripts

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

30

If you're familiar with computer programming, you'll probably have already come across the concept of functions in whatever programming languages you are familiar with. The advantages of using shell functions are basically the same as the advantages of using functions in a programming language, as you can probably tell from the slide above.

version: Lent 2020 29 Version: Lent 2020 30

Script as a series of functions

If you've implemented your shell script entirely as shell functions, there is a really nice trick you can use when something goes wrong and you need to debug your script, or if you want to re-use some of those functions in another script. As you've implemented the script entirely as a series of functions, you have to call one of those functions to start the script actually doing anything. For the purposes of this discussion, let's call that function main. So your script looks something like that shown on the slide above. (You can see an example of a script like this in the examples directory in the file function-script.)

scientific-computing@uis.cam.ac.uk

By commenting out the call to the **main** function, you now have a shell script that does *nothing* except define some functions. You can now easily call the function(s) you want to debug/use from another shell script using the **source** shell builtin command (as we'll see on the optional final day of this course). This makes debugging *much* easier than it otherwise might be, even of really long and complex scripts.

Improving multi-run

- Depends on run-once
- Location of **run-once** hard-coded into script:
 - If we move run-once, script breaks until it is updated

```
File: scripts/multi-run

#!/bin/bash

# Parameters that stay the same each run
fixed_parameters="0.005 0.0175 0.01 0.01"

# Run zombie program once for each argument
# Note: *no* quotes around $fixed_parameters
# or they'll be interpreted as one argument!
for population in "$@"; do
    "$HOME/scripts/run-once" $fixed_parameters "$population"
done

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two 32
```

On the previous day of this course we met the scripts multi-run and runonce. Together, these scripts gave us a nice way of running a program several times with different parameter sets. However, they are not as versatile as we might hope. run-once requires that the program it runs (zombie) be in the current directory. Since, in this example, zombie is a special program for us (imagine it were your program that you had written from scratch), that's not such a bad limitation, since we quite probably would have a working copy of the program in the directory where we were going to store its output.

multi-run, on the other hand, depends on the run-once script, and has the location of that script *hard-coded* into it. If we move the run-once script for some reason, then multi-run will immediately stop working. Wouldn't it be nice if we could somehow avoid this problem, but still keep the functionality of the two scripts somewhat separate?

One of way of doing exactly that would be to incorporate run-once into multi-run as a shell function. That should be quite easy. We define a function in multi-run that does *exactly* the same thing as the run-once script, and in our for loop, instead of calling the run-once script, we call our function.

So, let's do that and see what happens.

version: Lent 2020 31 version: Lent 2020 32

First exercise



Add run-once to multi-run

as a shell function:

```
# Run zombie program once for each argument
# Note: *no* quotes around ${fixed_parameters}

# Run zombie program once for each argument
# Note: *no* quotes around ${fixed_parameters}
# or they'll be interpreted as one argument!
for population in "$@"; do
run_program $fixed_parameters "$population"
done

# Simple Shell Scripting for Scientists: Day Two

33
```

The multi-run and run-once shell scripts are in the scripts directory of your home directory.

Your task is to get the functionality of the run-once script into the multi-run script as a shell function. (Hint: it's essentially a cut-and-paste exercise)

Above I've given you the skeleton of what the modified script should look like. You should be able to fill in the rest.

You can check that you've done it correctly by trying to run your modified multirun script (remember to save it after you've made your modifications!):

```
$ cd
$ rm -f *.dat stdout-* logfile
$ ls
$ scripts/multi-run 50 100 500 1000 3000 5000 10000 50000
$ ls
```

This should be a quick exercise, so when you finish it, take a short break and then we'll start again with the solution.

Recap: Shell functions

- "mini-shell scripts"
- Usually used for well-defined tasks (often called repeatedly)
- Specify arguments by listing them after function name when calling function hello Dave
- Positional parameters (and related special shell parameters) set to function's arguments within function

In function hello, positional parameter **1** = Dave

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

34

One thing worth noticing from the exercise we've just done:

```
The original script had the line:
```

```
"${HOME}/scripts/run-once" ${fixed_parameters} "${population}"
```

The new script has the line:

```
run_program ${fixed_parameters} "${population}"
```

Note that arguments that we are passing have not changed in the slightest. In the original script we were calling another shell script with some arguments. In our new script we are calling a *shell function* with the *same* arguments. The syntax for these is almost identical: the main change is the name (and location) of the things being called. See?, I told you shell functions were like "mini-shell scripts". \odot

Version: Lent 2020 33 Version: Lent 2020 34

Testing

```
#!/bin/bash

function run_program()
{
# This function runs the zombie program
...
}

# Parameters that stay the same each run
fixed_parameters="0.005 0.0175 0.01 0.01"

run_program $fixed_parameters 80

# Run zombie program once for each argument
# Note: *no* quotes around $fixed_parameters
# or they'll be interpreted as one argument!
#for population in "$@" ; do
# run_program $fixed_parameters "$population"
#done

scientific-computing@uis.cam.ac.uk Simple Shell Scripting for Scientists: Day Two
```

One of the advantages of writing a shell script using shell functions should be immediately apparent. The main body of this shell script – the **for** loop – is nice and simple. It just calls a function over and over varying one parameter each time. Because we've hidden the commands that do the real work in a shell function, we can see this immediately just by looking at the script.

If we'd put all the lines in the <code>run_program</code> function in the <code>for</code> loop it would have obscured the script's structure, and we might have spent a lot of time trying to figure out what the individual lines of script did before realising what was going on. It also helps that we've chosen a meaningful name for our shell function. So just by looking at the script we can immediately say "Aha! This script probably runs a program (<code>run_program</code>) several times, varying one of its parameters each time." (Of course, at this point we'd be taking it on faith that the author of the shell script wasn't an evil troll who deliberately chose <code>misleading</code> names for his shell functions. Fortunately, most of those spend the majority of their time under bridges harassing qoats.)

Another advantage is that we can easily test our shell function by just commenting the other complicating bits of the shell script out (as above) and just running the function once with some test arguments. This is worth doing every time you've written a new function (especially if it is complicated) so that you know it behaves the way you expected it to. It also means that you know that, if there is an error, it is *not* in that part of the shell script (that shell function). That makes it much easier to track down errors.

You can save the above modifications and try out the script if you want: it should just run the run_program function once, producing two output files (zombie-80.dat and stdout-80) and writing some information about what it is doing to the log file logfile.

If you do try it out, make sure that you undo those modifications and return the shell script to its former state (and save it) as we will be using the shell script later.

Command substitution

Sometimes we want to get the output of a command and use it in our shell script, for instance, we might want a shell variable to hold the output of a command. How do we do this?:

```
$( command )

$ cd /tmp
$ dir="$(pwd)"
$ echo "I will use directory: $dir"
I will use directory: /tmp
```

Command substitution is the process whereby the shell runs a command and substitutes the command's output for wherever the command originally appeared (in a shell script or on the command line).

So, for example, the following line in a shell script:

```
starting_directory="$(pwd)"
```

would set the shell variable **starting_directory** to the full path of the current working directory. (We don't have to surround the **\$(pwd)** in quotes, but it is a good idea: the path may contain spaces.) This is how it works:

- The shell runs the pwd command. The pwd command prints out the full path of the current working directory, i.e. its *output* is the full path of the current working directory. Let's suppose we were in /tmp, so the output of the pwd command would be "/tmp".
- 2. The shell takes this output ("/tmp") and substitutes it for where the original expression \$(pwd) appeared. So what we now have is:

```
starting_directory="/tmp"
```

3. As you probably know by now, this is just the normal way of assigning a value to a shell variable, and, sure enough, that's exactly what the shell does: it assigns the value "/tmp" to the shell variable starting_directory.

Instead of the **\$()** construct you can also use *backquotes*, i.e. you can use `*command*` instead of **\$(***command***)**, and you are likely to come across these in many shell scripts. However, the use of backquotes is generally a very bad idea for two reasons: (1) it's very easy to misplace or overlook a backquote (with catastrophic results) as the backquote character (`) is so small, and (2) it's very difficult to use backquotes to do *nested* command substitution (one command substitution inside another one).

Version: Lent 2020 35 Version: Lent 2020 36

Improving multi-run (2)

```
File: scripts/multi-run
#!/bin/bash

# Program to run: zombie
program="$(pwd)/zombie"

# Set up environment variables for program
export ZOMBIE_FORMAT="NORMAL"

# Parameters that stay the same each run
fixed_parameters="0.005 0.0175 0.01 0.01"

function run_program()
{

# Run program with passed arguments
"$program" "$@" > "stdout-${5}"

...
}
scientific_computing@uis.cam.ac.uk
Simple Shell Scripting for Scientists: Day Two
```

Let's make a small, but major, improvement to the multi-run script (this script is in the scripts directory of your home directory). Change the lines:

```
# Run zombie with passed arguments
ZOMBIE_FORMAT="NORMAL" ./zombie "${@}" > "stdout-${5}"
to:
# Run program with passed arguments
"${program}" "${@}" > "stdout-${5}"
And add the lines:
# Program to run: zombie
program="$(pwd)/zombie"

# Set up environment variables for program
export ZOMBIE_FORMAT="NORMAL"
immediately before the line:
# Parameters that stay the same each run
```

Why is this such a major improvement?

Firstly, by replacing the hard-coded ./zombie with a shell variable, we have made it much easier to modify the script to use other programs instead of zombie. (Not to mention making it much more obvious where we make such a modification. And by explicitly setting the ZOMBIE_FORMAT environment variable in an adjacent part of the script we have also made it more obvious where any environment variables the program uses should be changed, should we need to do so.)

Secondly, by obtaining the full path of the **zombie** program our shell script can now work in another directory than the one we start off in, as we now have a full path to the **zombie** program and so can run it from whatever directory we may be in. We'll see why this is a good idea in a minute.

You should check that this modified multi-run script still works – remember to save it after you've made your modifications – with the same sequence of commands given for this purpose on the page 33 of your notes.

The **mktemp** command

Safely makes temporary files or directories for you

Options:

- d make a directory instead of a file
- t make file or directory in a temporary directory (usually / tmp)

\$ mktemp -d -t zombie.XXXXXXXXX
/tmp/zombie.khhcE30735

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

38

The mktemp command is an extremely useful command that allows users to safely create temporary files or directories on multi-user systems. It is very easy to unsafely create a temporary file or directory to work with from a shell script, and, indeed, if your shell script tries to create its own temporary files or directories using the normal Unix commands then it is almost certainly doing so unsafely. Use the mktemp command instead.

Note that if you try the example above you will almost certainly get a directory with a different name created for you.

Note also that **mktemp** has more options than the two listed above, but we won't be using them in this course.

How do you use mktemp? You give it a "template" which consists of a name with some number of X's appended to it (note that is an UPPER CASE letter X), e.g. zombie.XXXXX. mktemp then replaces the X's with random letters and numbers to make the name unique and creates the requested file or directory. It outputs the name of the file or directory it has created.

Improving multi-run (3a)

```
#!/bin/bash
    # My current directory
    starting_directory="$(pwd)"
    # Temporary directory for me to work in
    temp_directory="$(mktemp -t -d zombie.XXXXXXXXX)"
    # Change to temporary directory
    cd "$temporary directory"
    # Run program once for each argument
    # Note: *no* quotes around $fixed_parameters
             or they'll be interpreted as one argument!
    for population in "$@"; do
      run_program $fixed_parameters "$population"
    # Copy files back to my directory
    cp -f -p -R . "$starting directory"
    # Go back to my directory
    cd "$starting_directory"
    # Clean up
    rm -R -f "$temp_directory"
scientific-computing@uis.cam.ac.uk
                              Simple Shell Scripting for Scientists: Day Two
                                                                               39
```

Modify the multi-run script in the scripts directory as shown above.

The improvement we've made here is to now do all our calculations in a temporary directory, and only copy the output files (and log file) back to our working directory when we've finished.

(You should understand what all the lines of shell script we've just added are doing – if you don't please ask the course giver or demonstrator to explain.)

Why is this an improvement? Well, if, as in this course, the directory we are working from (our home directory) is actually on a network filesystem, then this can have a major impact on performance, particularly when the network is busy (like when a whole classroom is doing this course). By working in /tmp, which is usually a local filesystem (as it is for MCS Linux machines) we no longer have to deal with the network overheads and bottlenecks except right at the very end of the process. This should make things much quicker. It also potentially makes things more reliable as well, as it minimises the opportunity for network problems to mess up our work. (Hurrah!)

One other important thing to note is that we've told our script to abort as soon as it hits an error. That's what adding the "set -e" line immediately after "#!/bin/bash" at the start of the file does (you did remember to make that modification, right?). (We can also get the same effect by starting the bash shell with the -e option, for instance by changing the "#!/bin/bash" line at the start of the file to "#!/bin/bash -e" although it is better to use "set -e".)

Why do this now? The reason is that our shell script is now doing something dangerous: *it is changing the working directory*. Why is that dangerous? Well, imagine I tried to change to a directory and failed for some reason. Thinking I'm in a different directory than I actually am, I promptly delete everything in it. Oops!

We have one more change to make (see the next slide) and then you can check that you've modified your script correctly by trying to run your modified multi-run script (remember to save it after you've made your modifications!).

Improving multi-run (3b)

```
File: scripts/multi-run
    #!/bin/bash
    set -e
    # Mv current directory
    starting_directory="$(pwd)"
    # Location of log file
     log_file="$starting_directory/logfile"
     function run_program()
       # Write to logfile
      echo "" >> "$log file"
       date >> "$log_file"
       echo "Running $program with $@" >> "$log_file"
      # Write to logfile
       echo "Output file: zombie-$5.dat" >> "$log file"
       echo "Standard output: stdout-$5" >> "$log file"
scientific-computing@uis.cam.ac.uk
                               Simple Shell Scripting for Scientists: Day Two
                                                                                 40
```

Now modify the multi-run script in the scripts directory as shown above.

We've made two improvements here. The first is to use a shell variable to hold the location of our log file (so we only have to change its location in one place in the future). The second (and more important) is to make our script write to the end of the existing logfile in the current directory when we run the script rather than *overwriting* logfile each time we run the script. Since the log file is supposed to contain a record of *all* the runs of the script that we do for posterity (and debugging), we normally wouldn't want it to be replaced with a new log file each time we run the script.

(You should understand what all the lines of shell script we've just added are doing – if you don't please ask the course giver or demonstrator to explain.)

You can check that you've done it correctly by trying to run your modified multi-run script (remember to save it after you've made your modifications!):

```
$ cd
$ rm -f *.dat stdout-*
$ ls
$ scripts/multi-run 50 100 500 1000 3000 5000 10000 50000
$ ls
```

Improving multi-run (3b)

```
File: scripts/multi-run
    #!/bin/bash
    set -e
    # Mv current directory
    starting_directory="$(pwd)"
    # Location of log file
    log_file="$starting_directory/logfile"
    function run_program()
      # Write to logfile
      echo "" >> "$log file"
      date >> "$log_file"
      echo "Running $program with $@" >> "$log_file"
      # Write to logfile
      echo "Output file: zombie-$5.dat" >> "$log file"
      echo "Standard output: stdout-$5" >> "$log file"
scientific-computing@uis.cam.ac.uk
                               Simple Shell Scripting for Scientists: Day Two
                                                                                 41
```

Now modify the multi-run script in the scripts directory as shown above.

We've made two improvements here. The first is to use a shell variable to hold the location of our log file (so we only have to change its location in one place in the future). The second (and more important) is to make our script write to the end of the existing logfile in the current directory when we run the script rather than *overwriting* logfile each time we run the script. Since the log file is supposed to contain a record of *all* the runs of the script that we do for posterity (and debugging), we normally wouldn't want it to be replaced with a new log file each time we run the script.

(You should understand what all the lines of shell script we've just added are doing – if you don't please ask the course giver or demonstrator to explain.)

You can check that you've done it correctly by trying to run your modified multi-run script (remember to save it after you've made your modifications!):

```
$ cd
$ rm -f *.dat stdout-*
$ ls
$ scripts/multi-run 50 100 500 1000 3000 5000 10000 50000
$ ls
```

Second Exercise



Make the changes to multi-run indicated on the previous slides (37, 39 & 40) and then *try* the improved script.

Then take a short break. We'll start again in 8 minutes or thereabouts.

8 minutes

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

42

The multi-run shell script is in the scripts directory of your home directory. Make the modifications indicated on the previous slides (37, 39 & 40), if you haven't already.

Now check that you've done it correctly by trying to run your modified multi-run script (remember to save it after you've made your modifications!):

```
$ cd
$ rm -f *.dat stdout-*
$ ls
$ scripts/multi-run 50 100 500 1000 3000 5000 10000 50000
$ ls
```

And when you finish doing this, please do take a quick break before we continue. (And that's "break" as in "break from the computer" not "break to check my e-mail".)

Version: Lent 2020 41 Version: Lent 2020 42

read

Get input from standard input...

...try to put each word (value) in as many separate variables as are provided...

read var1 var2 var3

Options:

- p Use the following string as a prompt for the user

```
$ read -p "What is the answer?: " answer
What is the answer?: 42
$ echo "$answer"
42
```

scientific-computing@uis.cam.ac.u

Simple Shell Scripting for Scientists: Day Two

The **read** shell builtin command takes input from standard input (usually the keyboard) and returns it in the specified shell variable. If you don't specify a shell variable, it will return it in a shell variable called **REPLY**.

The **-p** option gives **read** a string that it displays as a prompt for the user.

You can give **read** more than one shell variable in which to return its input. What happens then is that the first *word* it reads goes into the first shell variable, the second word into the second shell variable and so on.

If there are more words than shell variables, the extra words all are put into the last shell variable.

If there are more shell variables than words, each of the extra variables are set to the empty string.

As far as **read** is concerned a "word" is a sequence of characters that does *not* contain a space, i.e. it considers spaces as the thing that separates one word from another. (The technical term for "thing that separates one thing from another" is "delimiter".)

Using read (1)

```
$ cd
$ gedit scripts/run-once-using-read &

#!/bin/bash

# Read in parameters from standard input
read -p "Input parameters for zombie: " alpha beta zeta delta population
...

$ cd
$ scripts/run-once-using-read
Input parameters for zombie: 0.5 0.1 0.1 70
$
```

In the scripts directory there is a shell script called **run-once-using-read**. Open this up with your favourite editor (or gedit) and have a look at it.

The first line (that doesn't start with a # character) is a **read** shell builtin command that reads some values from standard input and puts them in some shell variables. (You should be able to work out how the rest of the script has been modified to use these shell variables – if there is anything you don't understand, ask the course giver or demonstrator.)

Let's try this script out and see how it behaves.

Version: Lent 2020 43 Version: Lent 2020 44

Using read (2)

```
$ cd
$ rm -f *.dat stdout-* logfile *.png
$ scripts/run-once-using-read
Input parameters for zombie: 0.5 0.1 0.1 70 garbage
Traceback (most recent call last):
 File "zombie", line 101, in <module>
    N0 = long(sys.argv[5])
ValueError: invalid literal for long() with base 10: '70 garbage'
mv: cannot stat `zombie.dat': No such file or directory
$ gedit scripts/run-once-using-read &
#!/bin/bash
# Read in parameters from standard input
read -p "Input parameters for zombie: " alpha beta zeta delta population junk
 scientific-computing@uis.cam.ac.uk
                            Simple Shell Scripting for Scientists: Day Two
                                                                       45
```

So, on first try it seemed to do what we'd expect. However, if we give it some input that should be invalid something slightly strange happens. If we give it 6 input parameters instead of 5, instead of complaining, or only using the first 5 parameters, it puts the last two parameters together to form one argument ("70 garbage") in the above example and runs the **zombie** program with that (we can see this is what is happening by inspecting the contents of the log file logfile). This causes the **zombie** program to crash with an error message that is less clear than one might hope (an indication that the **zombie** program is (yet again) not as well written as we might like (an all too common complaint with software)). (Also, as a result of **zombie** crashing, the **mv** command our shell script uses to rename zombie.dat file then complains that there is no file for it to rename.)

Regardless of how well or badly the **zombie** program handles invalid parameters, that fact that our script gives it mangled input to work with is an indication that our script is broken. What is the problem and how can we fix it?

Recall how **read** works: if it reads more words (values) than it was given shell variables, it puts all the extra ones together in the last shell variable. This is what is happening here, and it is undesirable. We can fix this by giving **read** an extra "dummy" shell variable that we never use, but that is simply there to hold any extra junk it may read in.

Modify the run-once-using-read shell script in the scripts directory as Nersion Showing above (remember to save it when you've finished).

Using read (3)

```
$ cd
$ rm -f *.dat stdout-* logfile
$ scripts/run-once-using-read
Input parameters for zombie: 0.5 0.1 0.1 70 garbage
$ ls
answers
        gnuplot
                        zombie.gplt
                                         scripts
         hello-function logfile
                                         source
        hello
                        zombie-70.dat
Desktop
                                         stdout-70
                        run-zombie
examples zombie
                                         treasure.txt
scientific-computing@uis.cam.ac.uk
                           Simple Shell Scripting for Scientists: Day Two
                                                                    46
```

Now it works better. If we give it more than 5 input parameters it doesn't mangle the 5th argument that it passes to the **zombie** program.

(Note that the output of the ls command may not exactly match what is shown above – in particular there may be other files or directories show, and the colours may be slightly different.)

Now this may seem like a lot of trouble to go to for not much in the way of improvement to our script. After all, the original run-once script could perfectly well accept a single set of 5 parameters without all these problems – it just wanted them on the command line rather than from standard input.

So, what's the big deal about standard input? After all, if I have lots of parameter sets to run I'm hardly going to sit there and type them all in one at a time!

Well, how many command line arguments can a shell script have? The answer is quite a few but *not* an unlimited number. In fact, If I have thousands of parameter sets, that's definitely going to be too many for me to pass to my shell script all in one go (or even a small number of goes) on the command line. So, how do we deal with situation?

Hmmmm, maybe if I could put all my thousands of parameter sets into a file, and then could somehow get my shell script to read in that file, one parameter set at at time, that might do it... we need to be able to do a few more things to make that particular idea fly, so let's have a look at some of them now...

45 Version: Lent 2020 46

Pipes

A pipe takes the

- ...output of one command...
- ...and passes it to another command as input...

command1 | command2

Pipes can be combined:

command1 | command2 | command3

A set of one or more pipes is known as a *pipeline*

scientific-computing@uis.cam.ac.ul

Simple Shell Scripting for Scientists: Day Two

A *pipe* takes the *output* of one command and feeds it to another command as *input*. We tell the shell to do this using the | symbol. So:

ls | less

takes the the output of the **ls** command and passes it to the **more** command, which displays the output of the **ls** command one screenful at a time. We can combine several pipes by taking the output of the last command of each pipe and passing it to the first command in the next pipe, e.g.

ls | grep 'fred' | less

takes the output of **ls** and passes it to **grep**, which searches for lines with the string "fred" in them, and then the output of **grep** is passed to the **less** command to display one screenful at a time. A set of one or more pipes is known as a *pipeline*. This pipeline would show us all the files with the string "fred" in their name, one screenful at a time.

Using pipes

```
$ rm -f *.dat stdout-* logfile
  $ cat scripts/basic param set
  0.005 0.0175 0.01 0.01 50
 0.005 0.0175 0.01 0.01 100
 0.005 0.0175 0.01 0.01 500
  0.005 0.0175 0.01 0.01 1000
 0.005 0.0175 0.01 0.01 3000
 0.005 0.0175 0.01 0.01 5000
 0.005 0.0175 0.01 0.01 10000
 0.005 0.0175 0.01 0.01 30000
 0.005 0.0175 0.01 0.01 50000
 0.005 0.0175 0.01 0.01 500000
 $ cat scripts/basic_param_set | scripts/run-once-using-read
 $ 1s
  answers
                            zombie.gplt
           anuplot
                                             scripts
            hello-function logfile
  hin
                                             source
 Desktop
          hello
                            zombie-50.dat
                                             stdout-50
 examples zombie
                            run-zombie
                                             treasure.txt
scientific-computing@uis.cam.ac.uk
                                Simple Shell Scripting for Scientists: Day Two
                                                                                  48
```

In the scripts directory there is a file called basic_param_set that contains a number of parameter sets. We can use the **cat** command to display the contents of this file. In fact, if we use the **cat** command on this file, the *output* of the **cat** command will be a list of parameter sets...

...and our run-once-using-read shell script will accept a complete parameter set as its *input*, so...

...if we connect the *output* of the cat command to the *input* of our shell script – by, say, using a pipe – maybe that will give us what we want? Let's try it!

Well, it almost does!, i.e. it does it for the first parameter set, but none of the others. If we try running it again and again it will still only do it for the first parameter set in the file, so we're not quite there, but close. What we want is some way of telling the script to keep reading until there is no more stuff to read.

In fact, what we want is for the script to do some sort of *loop*: reading in a set of values, then running the **zombie** program, then reading in the next set of values, and so on. How can we get it to do that? Before we look at that, we need to understand something else first...

Version: Lent 2020 47 Version: Lent 2020 48

Exit Status (1)

- Every program (or shell builtin command) returns an *exit status* when it completes
- Number between 0 and 255
- Not the same as the program's (or shell builtin command's) output
- By convention:
 - 0 means the command succeeded
 - Non-zero value means the command failed
- Exit status of the last command run stored in special shell parameter named?

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

The exit status of a program is also called its *exit code*, *return code*, *return status*, *error code*, *error status*, *errorlevel* or *error level*.

Exit Status (2)

```
gnuplot
                          zombie.qplt
                                          scripts
           hello-function logfile
                                          source
                                          stdout-70
 Desktop hello
                          zombie-70.dat
 examples zombie
                          run-zombie
                                          treasure.txt
 $ echo $?
 $ ls zzzz
 /bin/ls: zzzz: No such file or directory
 $ echo $?
scientific-computing@uis.cam.ac.uk
                          Simple Shell Scripting for Scientists: Day Two
```

You get the value of the special parameter? by using the construct \${?}, as in the above example.

Note that when the **ls** command is successful, its exit status is 0. When, however, it fails (for example because the file does not exist, as here), its exit status is non-zero ("2", in this case). In our shell scripts, we will make significant use of the fact that a non-zero exit status of a program (or a shell builtin command) means that there was an error.

Please note that the output of the **ls** command may not exactly match what is shown on this slide – in particular, the colours may be slightly different shades and there may be additional files and/or directories shown (and/or – if you've recently cleaned up your home directory – you may not have all of the files shown here).

version: Lent 2020 49 version: Lent 2020 50

true, false true do nothing, successfully \$ true \$ echo \$? 0 false do nothing, unsuccessfully \$ false \$ echo \$? 1

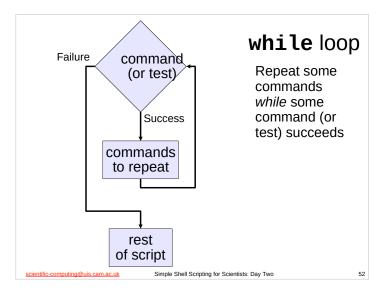
It's worth introducing a couple of commands at this point which do nothing. (No, really.)

true does nothing and always succeeds, i.e. its exit status of 0.

false does nothing and always **fails**, i.e. its exit status is non-zero.

You may be wondering what possible use there could be for such commands. The most obvious use is for debugging: suppose you have a script that runs a program that take a long time, and you want to test the script to make sure it works. You could replace the program that takes a long time with **true** to see what your script does if it thinks the program has succeeded. Similarly, you could replace the program your script is calling with **false** if you want to see what your script will do if it thinks the program has failed.

Another use for **true** is when you want the shell to do nothing (this is known as a *NOP* or *no-op* command): for instance, shell functions and **for** loops must contain at least one command. If, for some reason, you want a shell function or a **for** loop that does nothing (maybe because you haven't gotten around to writing it yet but you want to be able to test the rest of your script) you can use **true**. Then the shell won't complain about the definition of your function or the syntax of your **for** loop being incorrect, but they won't actually do anything.



Now that we know about the exit status of a command we are ready to meet the loop structure alluded to earlier:

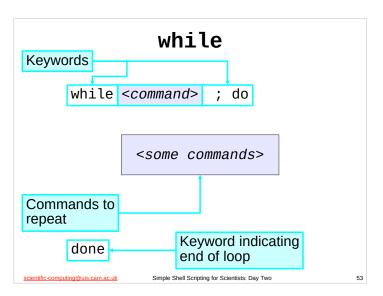
We can repeat a collection of one or more commands using a while loop. A while loop repeats a collection of commands as long as the result of some command is successful. The result of a command is considered to be successful if it returns an exit status of 0 (i.e. if the command succeeded). (The command we use in a while loop could also be a test of whether some expression is true. We'll see how to do that shortly.)

Note that even if set -e is in effect, or the first line of our shell script is

#!/bin/bash -e

the shell script will not exit if the result of the command the **while** loop depends on fails, since if it did, this would make **while** loops unusable(!).

version: Lent 2020 51 version: Lent 2020 52



We use a **while** loop like this:

while <command> ; do <some commands>

done

where **<command>** is a command (which could be a test: more on tests later), and <**some commands>** is a collection of one or more commands. Note that if <command> is false the shell script will not exit, even if set -e is in effect or the first line of the shell script is #!/bin/bash -e

As with a **for** loop, you can put the **do** on a separate line, in which case you can omit the semi-colon (;).

There are some examples of how to use **while** loops in the following files in the examples directory:

while1

while2

...but don't look at those files just yet as we need to meet a few more things first... Version: Lent 2020

while

Repeat *while* <command> returns *true*

while <command>; do <some commands> done

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

To recap: we can repeat a collection of commands using a while loop. A while loop repeats a collection of commands as long as the result of some command is true. The result of a command is considered to be true if it returns an exit status of 0 (i.e. if the command succeeded). (The command we use in a while loop could also be a test of whether some expression is true. We'll see how to do that shortly.) We use a while loop like this:

> while <command> ; do <some commands>

done

where <command> is a command (which could be a test), and <some commands> is a collection of one or more commands. Note that even if set -e is in effect, or the first line of the shell script is #!/bin/bash -e, the shell script will not exit if the result of <command> is not true.

As with a **for** loop, you can put the **do** on a separate line, in which case you can omit the semi-colon (;).

There are some examples of how to use while loops in the following files in the examples directory:

while1

while2

53

...but don't look at those files just yet as we need to meet a few more things first...

Version: Lent 2020

Using while (1)

```
$ cd
$ cp -p scripts/run-once-using-read scripts/run-while-read
$ gedit scripts/run-while-read &
File: scripts/run-while-read
#!/bin/bash

# Read in parameters from standard input
# and then run zombie with them
# and run it again and again until there are no more
while read -p "Input parameters for zombie: " \
    alpha beta zeta delta population junk; do
    ...
echo "Standard output: stdout-$population" >> logfile
done

scientific-computing@uis.cam.ac.uk
Simple Shell Scripting for Scientists: Day Two

55
```

Create a copy of the run-once-using-read shell script in the scripts directory called run-while-read. Open this up with your favourite editor (or gedit) and modify it as shown above.

Basically, replace the line:

 $\ensuremath{\text{read}}$ -p "Input parameters for zombie: " alpha beta zeta delta population junk

with:

```
# and then run zombie with them
# and run it again and again until there are no more
while read alpha beta zeta delta population ; do
```

And at the very end of the file add the following line: done

Remember to save the script when you've finished.

Now let's try this script out and see if it does what we want:

```
$ cd

$ rm -f *.dat stdout-* logfile

$ cat scripts/basic_param_set | scripts/run-while-read

$ ls
```

Third exercise

Make a copy of **multi-run** and read <u>all</u> the arguments for **zombie** in from standard input using a **while** loop:

```
$ cd
$ cp -p scripts/multi-run scripts/multi-run-while

File: scripts/multi-run-while

#!/bin/bash
set -e

# Run program once for each argument
# Note: *no* quotes around $fixed_parameters
# or they'll be interpreted as one argument!
for population in "$@" ; do
    run_program $fixed_parameters "$population"
done

10 minutes

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two
```

The multi-run shell scripts is in the scripts directory of your home directory. Make a copy of it called multi-run-while, also in the scripts directory, and work on that. Your task is to get multi-run-while to **read** in all the arguments for **zombie** from standard input (all its arguments, not just the fifth one) using a **while** loop.

Start by deleting the following two lines:

```
# Parameters that stay the same each run myFIXED_PARAMS="0.005 0.0175 0.01 0.01"
```

...and you should also get rid of any other references to the shell variable myFIXED_PARAMS – you won't be using it in this script.

We have gone through everything you need to do this exercise. You should comment the modifications you make to your shell script, preferably as you are writing it.

And when you finish this exercise, please do take a short break before we start again with the solution. (And that's "break" as in "break from the computer" not "break to check my e-mail".)

You can check that you've done it correctly by trying to run your multi-run-while script (remember to save it after you've made your modifications!):

```
$ cd
$ rm -f *.dat stdout-* logfile
$ ls
$ cat scripts/basic_param_set | scripts/multi-run-while
$ ls
```

Hint: Try copying the run-while-read script...
Version: Lent 2020

Recap: standard input/while loops

- Command substitution \$(command) can be used to get the output of a command into a shell variable
- Use mktemp to make temporary files and directories
- read gets values from standard input
- Pipes connect one command's output to another's input
- The command true does nothing but is considered to be true (its exit status is 0); the command false does nothing but is not considered to be true (non-zero exit status).
- while loops repeat some commands while something is true – can be used to read in multiple lines of input with read

scientific-computing@uis.cam.ac.u

Simple Shell Scripting for Scientists: Day Two

57

Note that **while** loops can contain other **while** loops, and they can also contain **for** loops (or both). Similarly, **for** loops can contain **while** loops or other **for** loops (or both).

Tests

```
Test to see if something
is true:
[[ <expression> ]]
```

```
[[ $a -eq $b ]]
[[ $a -le 42 ]]
[[ $a -gt 0 ]]
[[ $str = "aardvark" ]]
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

58

A test is basically the way in which the shell evaluates an expression to see if it is true. There are many different tests that you can do, and we only list a few here:

```
[[ $a -lt $b ]] true if and only if the integer a is less than the integer b
```

[[\$a -le \$b]] true if and only if the integer a is less than or equal to the integer b

[[\$a -eq \$b]] true if and only if the integer a is equal to the integer b

[[\$a -ne \$b]] true if and only if the integer a is not equal to the integer b

[[a -ge b]] true if and only if the integer a is greater than or equal to the integer b

[[\$a -gt \$b]] true if and only if the integer a is greater than the integer b

In the above tests, $\bf a$ and $\bf b$ can be any integers. Recall that shell variables can hold pretty much any value we like – they can certainly hold integer values, so $\bf a$ and/or $\bf b$ in the above expressions could come from shell variables, e.g.

```
[[ $VAR -eq 5 ]]
Or, equivalently:
```

test "\${VAR}" -eq "5"

is true if and only if the shell variable ${\it VAR}$ contains the value "5".

Note that you *must* have a space between the square brackets [[]]

N.B.: Use **-eq** for testing integers, and use **==** or **=** for testing the equality of strings.

N.B. Use **help test | less** to list the available tests and what they do.

Recap: Arithmetic Expansion \$(())

- Returns the value of an integer arithmetic operation
- Operands must be integers (so no decimals, e.g. 2.5, etc)
- Use bare variable names within the arithmetic expression

The shell can also do (primitive) integer arithmetic, which can be very useful.

Note that C syntax is used within the brackets, therefore you should use the bare variable name (This is, alas, inconsistent with the shell's behaviour elsewhere) We *can* put quotes around the entire arithmetic expansion construct, though, although this should not be necessary because the output should be numeric.

Use **help let** on the bash command line to find out what operations are available and how to use them.

while loops that count

Consider the following **while** loop:

```
counter=1
while [[ counter -le 6 ]] ; do
  echo $counter
  counter=$(( counter + 1 ))
done
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

60

When we put together arithmetic tests, **while** loops and arithmetic expansion, we can construct a **while** loop that counts for us, as in the above example. Can you figure out what the above loop will do?

When you think you know, try running the script while2 in the examples directory of your home directory. That will show you the output of the above while loop, immediately followed by the output of a very similar while loop where counter starts off with the value 0 rather than 1.

Note that **while** loops can (and often do) contain other **while** loops (or **for** loops). We say that one loop is *nested* inside the other one.

Using while (2)

```
$ cd
$ cat scripts/generate-params
#!/bin/bash
betas="0.0075 0.01 0.0175 0.0185 0.0195"
alpha=0.005
zeta=0.01
delta=0.01
for beta in $betas ; do
  population=50
  while [[ $population -le 50000 ]]; do
    echo "$alpha $beta $zeta $delta $population" >> new_param_set
    population=$(( population * 10 ))
  done
done
$ scripts/generate-params
$ more new_param_set
                              Simple Shell Scripting for Scientists: Day Two
                                                                              61
```

Examine the file called generate-params in the scripts directory of your home directory (shown above).

Then try it out and see what it does.

Generalising multi-run-while

```
File: scripts/multi-run-while

#!/bin/bash
set -e

"${program}" "${@}" > "stdout-$1-$2-$3-$4-$5"

mv zombie.dat "zombie-$1-$2-$3-$4-$5.dat"

echo "Output file: zombie-$1-$2-$3-$4-$5.dat" >> "${log_file}"
echo "Standard output: stdout-$1-$2-$3-$4-$5" >> "${log_file}"
```

Modify the multi-run-while script in the scripts directory as shown above.

(Remember to save it when you've finished.)

Basically we are replacing all the instances of the string " $\{5\}$ " with the string " $\{1\}-\{2\}-\{3\}-\{4\}-\{5\}$ ". This means that now, instead of our output files being based on the fifth argument that is passed to **zombie**, they are based on all the parameters in the parameter set. This is is clearly necessary as we start to experiment with varying parameters other than just the fifth one.

And we finish with an exercise.

If you want to do the exercise outside of class, the files you'll need can be found at:

https://help.uis.cam.ac.uk/help-support/training/downloads/ course-files/programming-student-files/shellscriptingsci/ shellscripting-files/exercises/day-two

Version: Lent 2020 61 Version: Lent 2020 62

If you're not coming back: Give us Feedback!

If, and only if, you will not be attending the next day of the course then please make sure that you fill in the Course Review form online, accessible under "feedback" on the main MCS Linux menu, or via:

http://feedback.training.cam.ac.uk/uis/

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

If you *are* coming to further sessions of this course, then you should fill in the feedback form at the **last** session you attend.

Final exercise – Part One

Improve the run_program function in multi-run-while so that as well as running zombie it also runs gnuplot (using the zombie.gplt file) to plot a graph of the output.

scientific-computing@uis.cam.ac.ul

Simple Shell Scripting for Scientists: Day Two

64

This exercise should be fairly straightforward. One sensible way of approaching it would be as follows:

- Figure out the full path of the zombie.gplt file. Store it in a shell variable (maybe called something like gnuplot_file).
- 2. Immediately after running zombie, run gnuplot:

gnuplot "\${gnuplot_file}"

3. Rename the zombie.png file produced by **gnuplot** along the same lines as the zombie.dat file produced by **zombie** is renamed.

Make sure you <u>test</u> the script after you've modified it and check that it does what you would expect.

This exercise highlights one of the advantages of using functions: we can improve or change our functions whilst leaving the rest of the script unchanged. In particular, the *structure* of the script remains unchanged. This means two things: (1) if there are any errors after changing the script they are almost certainly in the function we changed, and (2) the script is still doing the same *kind* of thing (as we can see at a glance) – we've just changed the particulars of one of its functions.

Version: Lent 2020 63 Version: Lent 2020 64

Final exercise – Part Two

Now create a new shell script based on multi-run-while that will run **zombie** three times for each parameter set the script reads in on standard input, changing the fifth parameter each time as follows:

For a given parameter set *a b c d e*, first your script should run **zombie** with the parameter set:

a b c d 50

...then with the parameter set:

a b c d **500**

...and then with the parameter set:

a b c d 5000

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

65

An example may help to make this task clearer. Suppose your script **read**s in the parameter set: 0.005 0.0175 0.01 0.01 70

...it should then run the zombie program 3 times, once for each of the following parameter sets:

0.005 0.0175 0.01 0.01 50 0.005 0.0175 0.01 0.01 500 0.005 0.0175 0.01 0.01 5000

The first thing to do is to make a copy of the multi-run-while script and work on the copy – I suggest you call your copy something like multi-50-500-5000:

\$ cc

\$ cp -p scripts/multi-run-while scripts/multi-50-500-5000

Now, currently the script will <code>read</code> in a parameter set and then call the <code>run_program</code> function to process that parameter set. Clearly, instead of passing all five parameters that the script reads in, your new script will now only be passing the first (<code>alpha</code>), second (<code>beta</code>), third (<code>zeta</code>), and fourth (<code>delta</code>) parameters that it has <code>read</code> in. However, the <code>zombie</code> program <code>requires</code> 5 parameters (and it cares about the order in which you give them to it), so your script still needs to give it 5 parameters, it is just going to <code>ignore</code> the fifth parameter it has <code>read</code> (<code>population</code>) and substitute values of its own instead.

There are two approaches you could take. One would be to call the <code>run_program</code> function 3 times, once with 50 as the fifth parameter, once with 500 as the fifth parameter and once with 5000 as the fifth parameter. The other would be to use some sort of loop that calls the <code>run_program</code> function, using the appropriate value (50, 500 or 5000) for the fifth parameter on each pass of the loop. I want you to use the loop approach.

Final exercise – Part Three

Now create a new shell script, based on the script you created in the previous part of the exercise, that does the following:

Instead of running **zombie** three times for each parameter set it **reads** in, this script should accept a set of values on the command line, and use those instead of the hard-coded 50, 500, 5000 previously used.

Thus, for each parameter set it reads in on standard input, it should run **zombie** substituting, in turn, the values from the command line **for** the fifth parameter in the parameter set it has **read** in.

So, if the script from the previous part of the exercise was called multi-50-500-5000, and we called this new script

multi-sizes (and stored both in the scripts directory of our home directory), then running the new script like this:

cd

\$ cat scripts/param_set | scripts/multi-sizes 50 500 5000

should produce $\it exactly$ the same output as running the old script with the same input file:

\$ cd

\$ cat scripts/param_set | scripts/multi-50-500-5000

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

66

The first thing to do is to make a copy of the previous script (which I suggested you call multi-50-500-5000) and work on the copy – I suggest you call your copy something like multi-sizes:

\$ cd

\$ cp -p scripts/multi-50-500-5000 scripts/multi-sizes

You may be wondering what the point of the previous script and this script are. Consider what these scripts actually do: they take a parameter set, vary one of its parameters and then run some program with the modified parameter sets. Why would we want to do this?

Well, in this example the parameter we are varying specifies the size of the population which our program will model. You can easily imagine that we might have a simulation or calculation for which, for any given parameter set, interesting things happened in various population sizes. These scripts allow us to take each parameter set and run it several times for different sizes of populations. We can then look at each parameter set and see how varying the size of the population affects the program's output for that parameter set.

If we were using the parameter sets in the scripts/param_set file, we might notice that these parameters are the same except for the second parameter which varies. So if we pipe those parameter sets into one of these scripts, we are now investigating how the output of the zombie program varies as we vary two of its input parameters, which is kinda neat, doncha think?

Output

Descripts/param_set file, we might notice that the second parameter which varies are the second parameter which is kinda neat, doncha think?

Hint: Modify the loop you used in the previous script to loop over all the command line arguments rather than some hard coded values. If you don't remember the construct that gives you all the command line arguments have a look at the recap of the previous day of this course.

Final exercise – Files



All the files (scripts, **zombie** program, etc) used in this course are available on-line at:

https://help.uis.cam.ac.uk/ help-support/training/downloads/ course-files/programming-student-files/ shellscriptingsci/shellscripting-files/ exercises/day-two

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Two

67

We'll be looking at the answers to this exercise on the next day of this course, so please make sure you have attempted this exercise **before** you come to the next day of this course.

Version: Lent 2020 67