

Simple Shell Scripting for Scientists

Day Three

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 considerably

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.

We finish at:

17:00

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

3

The course officially finishes at 17.00, so don't expect to finish before then. If you need to leave before 17.00 you 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.

Before the end of today's session, 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 Three

4

bash is probably 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>

Related course

Unix Systems: Further Commands:

- More advanced Unix/Linux commands you can use in your shell scripts
- Course discontinued (due to lack of demand) but course notes still available on-line

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

5

For the course notes from the “Unix Systems: Further Commands” course, see:

<https://help.uis.cam.ac.uk/help-support/training/downloads/course-files/programming-student-files/commands>

Outline of Course

1. Recap of days one & two
2. The **if** statement
3. **exit**, standard error

SHORT BREAK

4. More tests
5. **if...then...else**
6. Better error handling, **return**
7. **if...elif...elif...elif...else**

SHORT BREAK

8. Problems with **set -e**

Exercise

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

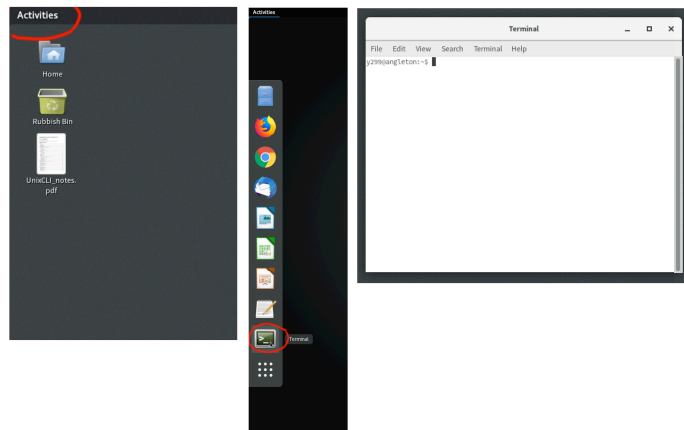
6

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.

Before the end of today's session, please make sure that you fill in the Course Review form online, accessible under “feedback” on the main MCS Linux menu, or via:

<https://feedback.training.cam.ac.uk/uis/>

Start a shell



scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

7

Recap: Days One & Two

- Shell scripts as linear lists of commands
- Simple use of shell variables and parameters
- Simple command line processing
- Shell functions
- Pipes and output redirection
- Accessing standard input using **read**
- **for** and **while** loops
- (Integer) arithmetic tests
- Command substitution and (integer) arithmetic expansion
- The **mktemp** command

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

8

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.

Recap: Shell functions (1)

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

$ ./hello-function
$
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

9

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.

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

```
function function_name()
```

```
{
```

where **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.

Recap: Shell functions (2)

- “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 Three

10

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:

```
function start()
{
    ...
}

function do_something()
{
    ...
}

function end()
{
    ...
}

function main()
{
    ...
}

main
```

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 the course). This makes debugging *much* easier than it otherwise might be, even of really long and complex scripts.

Recap: Output redirection and pipes

- Commands normally send their output to *standard output* (which is usually the screen)
- Standard output can be **redirected** to a file
- A **pipe** takes the *output* of one command and supplies it to another command as *input*.

Recap: More input and output, and **while** loops

- Command substitution **\$(command)** can be used to get the output of a command into a shell variable
- Use **mktemp** (see Appendix for details) to make temporary files and directories
- **read** gets values from standard input
- **while** loops repeat some commands while something is true – can be used to read in multiple lines of input with **read**
- A command is considered to be true if its *exit status* is 0.
- 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).

Note that even if we are using:

```
set -e
```

or the first line of our shell script is

```
#!/bin/bash -e
```

the shell script will not exit if the “something” the **while** loop depends on gives a non-zero exit status (i.e. is false), since if it did, this would make **while** loops unusable(!).

Recap: Exit Status

- 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 `?`

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

You get the value of the special parameter `?` by using the construct `${?}`.

Recap: Tests

Test to see if something is true:

```
[[ <expression> ]]
```

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

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, **a** and **b** can be any integers. Recall that shell variables can hold pretty much any value we like – they can certainly hold integer values, so **a** and/or **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 **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: Shell arithmetic

- The shell can do *integer* arithmetic – this is known as **arithmetic expansion**
- The shell can also perform arithmetic **tests** on integers (>, ≥, =, ≤, <)

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**

`$((<arithmetic-expression>))`

Example:

`$((VAR + 56))`

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

The construct **`$((<arithmetic-expression>))`** means replace **`$((<arithmetic-expression>))`** with the result of the *integer* arithmetic expression **`<arithmetic-expression>`**. This is known as *arithmetic expansion*. (The arithmetic expression is evaluated as integer arithmetic.)

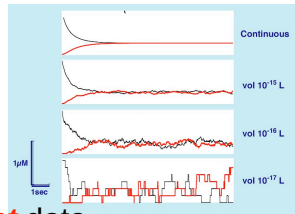
Note that C syntax is used within the brackets, therefore you should use the bare variable name (This is, alas, inconsistent with the shell's behaviour elsewhere) We *can* put quotes around the entire arithmetic expansion construct, though, although this should not be necessary because the output should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

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



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 first 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)

```
$ ./zombie 0.005 0.0175 0.01 0.01 500
```

When Zombies Attack!: Basic Model of outbreak of zombie infection

```
Population size:      5.00000e+05
Model run time:      1.0e+01 days

Zombie destruction rate (alpha):  5.000000e-03
Zombie infection rate (beta):    1.750000e-02
Zombie resurrection rate (zeta):  1.000000e-02
Natural death [and birth] rate (delta): 1.000000e-02

Output file:          zombie.dat

Model took 7.457018e-02 seconds
```

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.

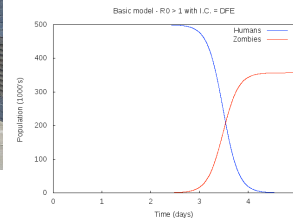
Sample program: **zombie** (2)

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



Photo: Melbourne Zombie Shuffle by Andrew Braithwaite
Licensed under CC BY 2.0
<http://www.flickr.com/photos/bratha/2578784637/>

blue = Humans
red = Zombies



scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

19

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している

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.

این صفحه خالی است

An leathanach seo fágtha folamh in aon turas.

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

20

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).

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. Tchuente & 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: nothing to see here.

Exercise from Day Two (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.

The **multi-run-while** shell script (in the **scripts** subdirectory of your home directory) runs the **zombie** program (via a shell function called **run_program**) once for each parameter set that it **reads** in from standard input. This exercise requires you to modify the **run_program** shell function of that script so that, as well as running the **zombie** program it also runs **gnuplot** to turn the output of the **zombie** program into a graph.

One sensible way of doing this would be as follows:

1. Figure out the full path of the **zombie.gplt** file. Store it 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.

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.

Solution to Part One

```
#!/bin/bash
set -e

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

# Location of gnuplot file
gnuplot_file="$(pwd -P)/zombie.gplt"

function run_program()
{
    # Run program with passed arguments
    "$program" "$@" > "stdout-$1-$2-$3-$4-$5"

    # Run gnuplot
    gnuplot "$gnuplot_file"

    # Rename files
    mv zombie.dat "zombie-$1-$2-$3-$4-$5.dat"
    mv zombie.png "zombie-$1-$2-$3-$4-$5.png"

    # Write to logfile
    echo "Output file: zombie-$1-$2-$3-$4-$5.dat" >> "$log_file"
    echo "Plot of output file: zombie-$1-$2-$3-$4-$5.png" >> "$log_file"
}
```

If you examine the **multi-run-while** script in the **scripts** subdirectory of your home directory, you will see that it has been modified as shown above to run **gnuplot** after running **zombie**.

You should be able to tell what all the highlighted parts of the shell script above do – if there is anything you don’t understand, or if you had any difficulty with this part of the exercise, please let the course giver or demonstrator know.

You can test that this script works by doing the following:

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

You should see that there is a PNG file for each of the renamed **.dat** output files. You should also inspect **logfile** to see what it looks like now.

Exercise from Day Two (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 Three

23

An example may help to make this task clearer. Suppose your script **reads** 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`

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

There are two obvious approaches you could have taken in performing this task. One would be to call the **run_program** 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 **run_program** function, using the appropriate value (50, 500 or 5000) for the fifth parameter on each pass of the loop. I wanted you to use the loop approach.

Solution to Part Two (1)

```
#!/bin/bash
set -e

...

# Sizes to use instead of read in value
populations="50 500 5000"

# Read in parameters from standard input
# and then run program with them
# and run it again and again until there are no more
while read alpha beta zeta delta junk ; do
    # Instead of using read in value for size,
    # use values from variable populations.
    # Note: *no* quotes around $populations or values will be
    # interpreted as a single value!
    for population in $populations ; do
        # Run program
        run_program "$alpha" "$beta" "$zeta" "$delta" "$population"
    done
done

...
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

24

If you examine the `multi-50-500-5000` script in the `scripts` subdirectory of your home directory, you will see that it is a version of the `multi-run-while` script that has been modified as shown above.

You should be able to tell what all the highlighted parts of the shell script above do, and you should be able to see why this is a solution to this part of the exercise – if there is anything you don't understand, or if you had any difficulty with this part of the exercise, please let the course giver or a demonstrator know.

You can test that this script works by doing the following:

```
$ cd
```

```
$ rm -f *.dat *.png stdout-* logfile
```

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

```
$ ls
```

You should see that a number of PNG and `.dat` files have been produced. You could view some of the PNG files to make sure they were what was expected by using Eye of GNOME (**eog**) or another PNG viewer (such as Firefox).

Solution to Part Two (2)

```
#!/bin/bash
set -e

...

# Read in parameters from standard input
# and then run program with them
# and run it again and again until there are no more
while read alpha beta zeta delta junk ; do
    # Instead of using read in value for size,
    # use 50, then 500, then 5000.
    population=50
    while [[ $population -le 5000 ]] ; do
        # Run program
        run_program "$alpha" "$beta" "$zeta" "$delta" "$population"
        population=$(( population * 10 ))
    done
done

...
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

25

There is another way you could have achieved the same thing, also using a loop, but this time using a **while** loop instead of a **for** loop. This may seem a somewhat perverse way of doing things, but if you had a parameter that was an integer that you wished to increase by some constant factor a large number of times, e.g. 2, 4, 8, 16, 32, 64, etc. then this would be a better way of doing it than trying to type them all out as a list of values for a **for** loop.

If you examine the `multi-50-500-5000-alternate` script in the `scripts` subdirectory of your home directory, you will see that it is a version of the `multi-run-while` script that has been modified as shown above.

You should be able to tell what all the highlighted parts of the shell script above do, and you should be able to see why this is a solution to this part of the exercise – if there is anything you don't understand, or if you had any difficulty with this part of the exercise, please let the course giver or a demonstrator know.

You can test that this script works by doing the following:

```
$ cd
$ rm -f *.dat *.png stdout-* logfile
$ cat scripts/param_set | scripts/multi-50-500-5000-alternate
$ ls
```

...and examining the files produced.

Exercise from Day Two (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 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 Three

26

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? ☺

Solution to Part Three

```
#!/bin/bash
set -e

...

# Read in parameters from standard input
# and then run program with them
# and run it again and again until there are no more
while read alpha beta zeta delta population junk ; do
    # Instead of using read in value for size,
    # cycle through command line arguments.
    for population in "$@" ; do
        # Run program
        run_program "$alpha" "$beta" "$zeta" "$delta" "$population"
    done
done

...
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

27

If you examine the `multi-sizes` script in the `scripts` subdirectory of your home directory, you will see that it is a version of the `multi-50-500-5000` script that has been modified as shown above.

You should be able to tell what all the highlighted parts of the shell script above do, and you should be able to see why this is a solution to this part of the exercise – if there is anything you don't understand, or if you had any difficulty with this part of the exercise, please let the course giver or a demonstrator know.

You can test that this script works by doing the following:

```
$ cd
$ rm -f *.dat *.png stdout-* logfile
$ cat scripts/param_set | scripts/multi-sizes 50 500 500
$ ls
```

You should see that a number of PNG and .dat files have been produced.

What else are tests good for?

We have seen that we can use tests in **while** loops. What else are they good for?

Suppose we know some (valid) parameters for our program produce no interesting output. Could we use some tests to filter these out?

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

28

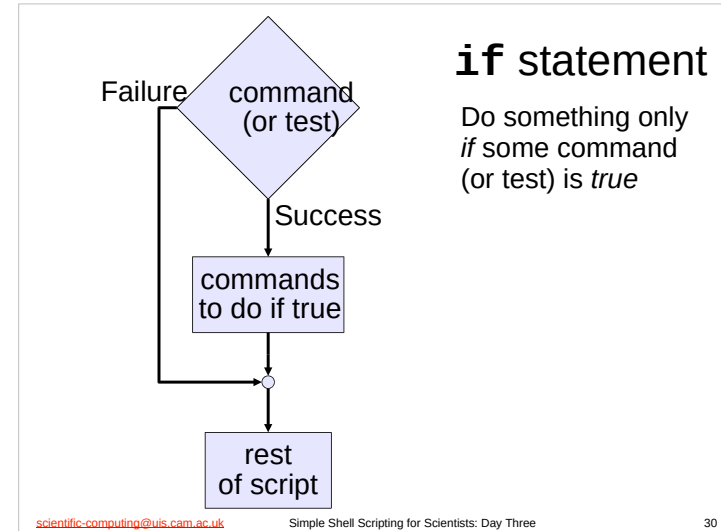
Using tests (1)

We've met (integer) arithmetic tests.

Suppose we'd like to test to see whether some of our parameters are within a certain range (say 1 to 1000000). If they are not, we shouldn't do anything, i.e.

If parameter < 1 or parameter > 1000000 stop executing the script...

How do we do this?



We can decide whether a collection of commands should be executed using an **if** statement. An **if** statement executes a collection of commands **if and only if** the result of some command or test is true. (Recall that the result of a command is considered to be true if it returns an exit status of 0 (i.e. if the command succeeded)).

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 or test the **if** statement depends on is false (i.e. it returns a non-zero exit status), since if it did, this would make **if** statements fairly useless(!).

if

Do something **only if** some command is *true*

```
if <command> ; then
    <some commands>
fi
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

31

We use an **if** statement like this:

```
if <command> ; then
    <some commands>
fi
```

where **<command>** is either a command or a test, 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`

In a similar manner to **for** and **while** loops, you can put the **then** on a separate line, in which case you can omit the semi-colon (;), i.e.

```
if <command>
then
    <some commands>
fi
```

Now, we just need to know how to tell our script to stop executing and we will have all the pieces we need to modify our script to behave the way we want...

exit

To stop executing a shell script:

exit

...can explicitly set an exit status thus:

exit value

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

32

The **exit** shell builtin command causes a shell script to *exit* (stop executing) and can also explicitly set the exit status of the shell script (if you specify a value for the exit status).

Recall that the exit status is an integer between 0 and 255, and should be 0 **only** if the script was successful in what it was trying to do. If the script encounters an error it should set the exit status to a non-zero value.

If you don't give **exit** an exit status then the exit status of the shell script will be the exit status of the last command executed by the script before it reached the **exit** shell builtin command.

(If you don't have an **exit** shell builtin command in your shell script, then your script will exit when it executes its last command. In this case its exit status will be the exit status of the last command executed by your script.)

Using `if` (and tests)

```
File: scripts/multi-sizes
#!/bin/bash
set -e

...

while read alpha beta zeta delta population junk ; do
# Instead of using read in value for size,
# cycle through command line arguments.
for population in "$@" ; do

    if [[ $population -lt 1 ]] ; then
echo "Size of population ($population) must be positive!"
exit 1
    fi
    if [[ $population -gt 1000000 ]] ; then
echo "Population ($population) too large!"
exit 1
    fi

# Run program

...


```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

33

Modify the `multi-sizes` script in the `scripts` subdirectory of your home directory as shown above. (Make sure to save it after you've modified it.)

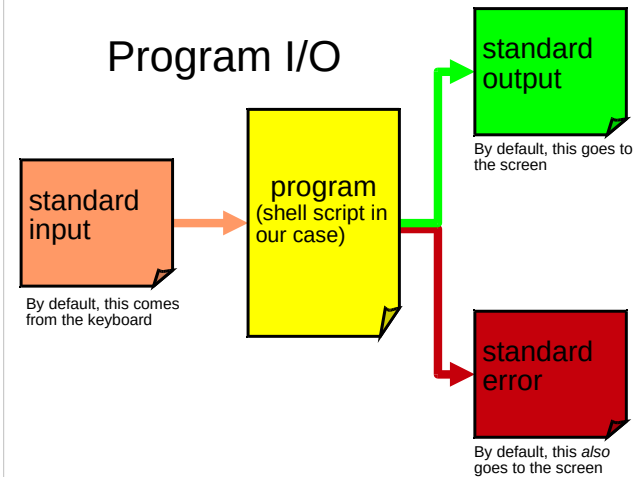
What do you think these modifications do?

Note that if we **exit** the script because one of the command line arguments is incorrect, then we need to indicate that there was a problem running the script, so we set our exit status to a non-zero value (1 in this case, which is the conventional value to use if we don't set different values for the exit status for different types of error).

You can test that this script works by doing the following:

```
$ cd
$ rm -f *.dat *.png stdout-* logfile
$ cat scripts/param_set | scripts/multi-sizes 0
Size of population (0) must be positive!
$ cat scripts/param_set | scripts/multi-sizes 2000000
Population (2000000) too large!
```

Program I/O



scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

34

We are already familiar with *standard output* as a “channel” along which our program or shell script’s output is sent to somewhere. By default, this “somewhere” will be the screen, unless we *redirect* it to somewhere else (like a file).

Standard output is one of the *standard streams* that all programs (whether they are shell scripts or not) have. (The idea of a *stream* here is that there is a “stream” of data flowing to/from our program and to/from somewhere else, like the screen.) Another standard stream that we have already met is standard input (which by default comes from the keyboard unless we redirect it).

There is actually a *third* standard stream called *standard error*. Like standard output, this is an “output stream” – data flows *from* our program along this stream *to* somewhere else. This stream is not for ordinary output though, but for any error messages our program may generate (and by default it also goes to the screen).

Why have two output streams? The reason is that this allows error messages to be easily separated from a program’s output, e.g. for ease of debugging, etc.

For more information on standard error and the other standard streams (standard input and standard output) see the following Wikipedia article:

https://en.wikipedia.org/wiki/Standard_streams

Standard Error (1)

```
$ ls zombie
zombie

$ ls zombie zzzzfred
/bin/ls: zzzzfred: No such file or directory
zombie

$ ls zombie zzzzfred > stdout-ls
/bin/ls: zzzzfred: No such file or directory

$ cat stdout-ls
zombie
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

35

If we look at what happens when a standard Unix command, such as **ls**, encounters an error, the way standard error works may become clearer.

When we ask **ls** to list a non-existent file, it prints out an error message. If we redirect the (standard) output of **ls** to a file, we see that the error message still goes to the screen. This is because the error message does not go to standard output, but to standard error. If we wanted to send the error message to file we would need to redirect *standard error* to that file.

So how do we manipulate standard 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.

Standard Error (2)

To redirect standard error to a file we use the following construct:

```
command 2> file
```

To send the output of a command to standard error, we use the following construct:

```
command >&2
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

36

Note that there is no space between the “2” and the “>” or the “>” and the “&2”, i.e.

it is	“2>”	not	“2 >”
and	“>&2”	not	“> &2” or “> & 2”

This is very important – if you put erroneous space characters in these constructs, the shell will not understand what you mean and will either produce an error message, or worse, do the wrong thing.

Using standard error

```
File scripts/multi-sizes
#!/bin/bash
set -e

...
while read alpha beta zeta delta junk ; do
# Instead of using read in value for size,
# cycle through command line arguments.
for population in "$@" ; do

    if [[ $population -lt 1 ]] ; then
echo "Size of population ($population) must be positive!" >&2
exit 1
    fi
    if [[ $population -gt 1000000 ]] ; then
echo "Population ($population) too large!" >&2
exit 1
    fi

# Run program

...

scientific-computing@uis.cam.ac.uk Simple Shell Scripting for Scientists: Day Three 37
```

Modify the `multi-sizes` script in the `scripts` subdirectory of your home directory as shown above. (Remember to save it after you've made the above changes or they won't take effect.)

Since when we exit the script because we don't like one of the parameters, we consider this an error, the message we print out telling the user what the problem is is an error message, and so should go to standard error rather than standard output. This is what adding `>&2` to those `echo` shell builtin commands does.

This is the conventional behaviour for shell scripts (or indeed any other program) – ordinary output goes to standard output, error messages go to standard error. It is *very important* that you follow this convention when writing your own shell scripts as this is what anyone else using them will expect them to do.

First exercise



The problem with the checking we've added to the `multi-sizes` script is that it will only stop as and when it encounters a bad parameter, so that it may start a run and then abort it part way through.

Write a function called `check_args` to check that each of its arguments is between 1 and 1000000. (You can assume that each argument is an integer.) Modify the script to use this function on *all* the command line arguments before it enters its `while` loop.

```
File scripts/multi-sizes
#!/bin/bash
set -e

...

function check_args()
{
# This function checks all the arguments it has been given
What goes here?
}

...

# Location of log file
log_file="$starting_directory/logfile"

# Make sure our command line arguments are okay before continuing
check_args "$@"

...

scientific-computing@uis.cam.ac.uk Simple Shell Scripting for Scientists: Day Three 38
```

⏪ 10 minutes

The `multi-sizes` shell script is in the `scripts` directory of your home directory. Your task is to add a shell function to this script that the script can use to check *all* the command line parameters it has been given to ensure they are between 1 and 1000000 (you can assume the parameters are integers), and then to modify the script to call that function before it does anything significant. Above I've given you the skeleton of what the modified script should look like. You should be able to fill in the rest. *Make sure you save your script after you've modified it.*

Note that you need to (re)move the `if` statements that we've added to the shell script as once we use the `check_args` function we will have already checked the command line arguments by the time we enter the `while` loop, and there is no point in checking them twice.

When you finish this exercise, take a short break and then we'll start again with the solution.

Note that in the skeleton above I call the `check_args` function *before* I use the `mktemp` command – there's no point in creating a temporary directory if I've been given bad parameters and am going to abort my script...

Hint: We've actually already written most of the function – so you can cut-and-paste those lines of the current shell script into the function. You then need to somehow *loop* through all the function's arguments, checking each in turn.

More tests (1)

Test to see if something is true:

```
[[ <expression> ]]
```

or: `test <expression>`

where *<expression>* can be any of a number of things such as:

```
[[ -z "$a" ]]
```

```
[[ "$a" = "$b" ]]
```

```
[[ -e "filename" ]]
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

39

As well as the (integer) arithmetic tests we have already met, there are a number of other tests we can do. They fall into two main categories: tests on files and tests on strings.

There are many different such tests and we only list a few of the most useful below:

<code>-z "a"</code>	true if and only if a is a string whose length is zero
<code>"a" = "b"</code>	true if and only if the string a is equal to the string b
<code>"a" == "b"</code>	true if and only if the string a is equal to the string b
<code>"a" != "b"</code>	true if and only if the string a is not equal to the string b
<code>-d "filename"</code>	true if and only if the file filename is a directory
<code>-e "filename"</code>	true if and only if the file filename exists
<code>-h "filename"</code>	true if and only if the file filename is a symbolic link
<code>-r "filename"</code>	true if and only if the file filename is readable
<code>-x "filename"</code>	true if and only if the file filename is executable

You can often omit the quotation marks but it is good practice to get into the habit of using them, since if the strings or file names have spaces in them then *not* using the quotation marks can be disastrous. (Note that string comparison is *always* done **case sensitively**, so “HELLO” is not the same as “hello”).

You can get a complete list of all the tests

looking in the CONDITIONAL EXPRESSIONS section of **bash**’s man page (type “**man bash**” at the shell prompt to show **bash**’s man page.)

More tests (2)

We can negate an expression, i.e. test to see whether the expression was false, using **!** thus:

```
[[ ! <expression> ]]
```

or: `test ! <expression>`

The above are true if and only if *<expression>* is *false*, e.g.

```
[[ ! -z "$a" ]]
```

is true if and only if \$a is a string whose length is *not* zero.

We can also use **!** with a command in an **if** statement or **while** loop to mean only do whatever the **if** or **while** is supposed to do if the command *fails* (i.e. its exit status is *not* 0).

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

40

Remember that in a **while** loop or an **if** statement we can use commands as well as tests. The command is considered true if it succeeds, i.e. its exit status is 0. In a **while** loop or an **if** statement we can negate a command in exactly the same way we negate *<expression>*, using **!** – negating a command means that the **while** loop or **if** statement will only consider it true if the command *fails*, i.e. its exit status is *non-zero*.

So:

```
while ! ls datafile ; do
    echo "Can't list file datafile!"
done
```

...would print the string “Can't list file datafile!” on the screen as long as **ls** was unable to list the file **datafile**, i.e. as long as the **ls** command returns an error when it tries to list the file **datafile** (for instance, if the file didn't exist).

Similarly:

```
if ! ./zombie ; then
    echo "Unable to run ./zombie successfully"
fi
```

...will only print the message “Unable to run ./zombie successfully” if the **zombie** program in the current directory returns a non-zero exit status (i.e. it fails for some reason).

N.B. `[[! -z $a]]` is equivalent to the test `[[-n $a]]`

Using tests (2)

```
File scripts/multi-sizes
#!/bin/bash
set -e

function check_args()
{
    # This function checks all the arguments it has been given

    # Make sure that we have some command line arguments.
    if [[ ${#} = 0 ]] ; then
        echo "No arguments given." >&2
        echo "This script takes one or more population sizes as its arguments." >&2
        echo "It requires at least one argument." >&2
        exit 1
    fi
    ...
}
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

41

Modify the `multi-sizes` script in the `scripts` subdirectory of your home directory as shown above. (Remember to save it after you've made the above changes or they won't take effect.)

Now we not only complain if we have arguments that are out of range, we also complain if we have no arguments at all (and also if our first argument is an empty string). Try this script out now and see what happens:

```
$ cd
```

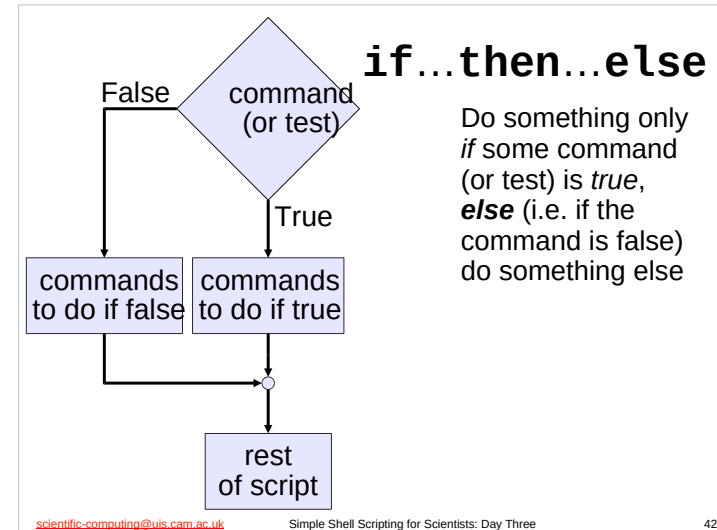
```
$ cat scripts/param_set | scripts/multi-sizes
```

```
Invalid argument or no arguments given.
```

```
This script takes one or more population sizes as its arguments.
```

```
It requires at least one argument.
```

Note also that we are once again making use of the fact that we have separated some functionality from our script and put it in a function. We can easily change the function without complicating the rest of the script or affecting its structure.



scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

42

As well as deciding whether a collection of commands should be executed at all, we can also decide whether one or other of two collections of commands should be executed using a more advanced form of the **if** statement. If there is an **else** section to an **if** statement the collection of commands in the **else** section will be executed *if and only if* the command (or test) we are evaluating is *false*.

if...then...else

Do something only *if* some command is true, **else** (i.e. if the command is false) do something else.

```
if <command> ; then
    <some commands>
else
    <some other commands>
fi
```

As well as deciding whether a collection of commands should be executed at all, we can also decide whether one or other of two collections of commands should be executed using a more advanced form of the **if** statement. If there is an **else** section to an **if** statement the collection of commands in the **else** section will be executed **if and only if** the given *<command>* is **false**. Note the syntax above.

Using if...then...else

```
File: scripts/multi-sizes
#!/bin/bash
set -e

...

function multi_sizes()
{
    # Instead of using read in value for size,
    # cycle through arguments passed to function.
    for population in "$@" ; do

        # Run program
        run_program "$alpha" "$beta" "$zeta" "$delta" "$population"
    done
}

...

while read alpha beta zeta delta population junk ; do
    if [[ $# = 0 ]] ; then
        # If there are no arguments then use these defaults
        echo "Using default population sizes: 50, 500, 5000"
        multi_sizes "50" "500" "5000"
    else
        # Use the command line arguments
        multi_sizes "$@"
    fi
done
```

Open up the `multi-sizes-default` script in the `scripts` subdirectory of your home directory in your favourite editor (or `gedit`) and have a look at it.

Notice that the **check_args** function in this script doesn't complain if there are no command line arguments. This is because this script will use some *default* parameters if it hasn't been given any on the command line. (And note that we print a message on the screen so the person using our script knows its using default values and *what those values are*.)

Pay particular attention to the bits of the script highlighted above. Can you work out what we've changed and how the shell script will now behave? If not, please tell the course giver or a demonstrator what part of the script you don't understand.

Try out this script and see what happens:

```
$ cd
$ rm -f *.dat *.png stdout-* logfile
$ cat scripts/param_set | scripts/multi-sizes-default
$ ls
```

Note that we didn't *need* to create a separate **multi_sizes** function – we could have just typed out very similar lines of shell script twice. This would have been a mistake – just like with real programming languages, repetition of parts of our script (program) are almost *always* to be avoided.

Better error handling (1)

At the moment, any errors stop our script dead. Often, that's better than letting it carry on regardless, but sometimes we want to be a bit more sophisticated.

For instance, supposing a few parameter sets we read in are corrupt and cause errors in **zombie** or **gnuplot** – we might want to note which ones these were and continue with the others.

How can we do this?

return

Just like programs and shell scripts have an exit status, so too do shell functions (although it is unwise to try and make significant use of these). We can set the exit status of a function using the **return** shell builtin command, and when we use **return** we should *always* explicitly set the exit status (normally to 0).

To stop executing a function and safely return to wherever we were called from, use:

```
return 0
```

...we can set a non-zero exit status as we exit the function thus (where *value* is between 1 and 255):

```
return value
```

The **return** shell builtin command causes a shell function to stop executing and return control to whatever part of the shell script called it. It can also explicitly set the exit status of the function, and when we use **return** we should explicitly set the status (normally to 0).

As with ordinary programs and shell scripts themselves, the exit status of a shell function is an integer between 0 and 255, and, as one might expect, the convention is that the exit status should be 0 only if the function was successful in what it was trying to do. Unfortunately, if the function returns a non-zero exit status, this can cause very subtle (i.e. difficult to track down) types of misbehaviour, so it is actually safest to always use **return** with an exit status of 0 (i.e. “**return 0**”).

(If you don't give **return** an exit status then the exit status of the shell function will be the exit status of the last command executed by the function before it reached the **return** shell builtin command, but this can lead to extremely subtle types of misbehaviour – use “**return 0**” instead.

And if you don't have a **return** shell builtin command in your shell function, then your function will exit when it executes its last command. In this case its exit status will be the exit status of the last command executed in your function – this can also cause subtle problems, so your functions should really always end with “**return 0**”).

Better error handling (2)

```
File: scripts/multi-sizes
#!/bin/bash
set -e

...

function multi_sizes()
{
# Instead of using read in value for size,
# cycle through arguments passed to function.

for population in "$@" ; do

# Assume parameter set will work
bad_parameter="0"

# Run program
run_program "Alpha" "Beta" "Zeta" "Delta" "Spopulation"

# Report if there were problems
if [[ $bad_parameter -gt 0 ]] ; then
echo "Problem with parameter set: Alpha Beta Zeta Delta Spopulation" >&2
fi

done
}

...
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

47

Open up the `multi-sizes-errors` script in the `scripts` subdirectory of your home directory in your favourite editor (or `gedit`) and have a look at it.

First have a look at the `multi_sizes` function, paying particular attention to the bits of the script highlighted above. Can you guess why we've changed this function like this?

If we look at the `run_program` function and see how that's been changed it should become clear why we've changed the `multi_sizes` function this way. First though, we need to learn how to toggle the shell's "quit on any error" behaviour on and off at will...

`set -e, set +e`

Abort shell script if an error occurs:

```
set -e
```

Abort shell script only if a syntax error is encountered (default):

```
set +e
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

48

We already know that if the first "magic" line of our shell script is:

```
#!/bin/bash -e
```

then the shell script will abort if it encounters an error. We also know we can make this happen by using `set -e` instead, if we prefer.

Sometimes though, we may want to handle errors ourselves, rather than just having our shell script fall over in a heap. So it would be nice if we could turn this behaviour off and on at the appropriate points in the shell script, and `bash` provides a mechanism for us to do just that:

- As we know, `set -e` tells the shell to quit when it encounters an error in the shell script. Whenever you are not doing your own *error handling* (i.e. checking to make sure the commands you run in your shell script have executed successfully), you *should* use `set -e`.
- `set +e` returns to the default behaviour of continuing to execute the shell script even after an error (other than a syntax error) has occurred.

A good practice to get into is to always have the following as the first line of your shell script that isn't a comment (i.e. doesn't start with a `#`):

```
set -e
```

and then to turn this behaviour off *only* when you are actually dealing with the errors yourself.

Better error handling (3)

```
File: scripts/multi-sizes
#!/bin/bash
set -e

...

function run_program()
{
    ...

    # Run program with passed arguments
    set +e
    "$program" "$@" > "stdout-$1-$2-$3-$4-$5"
    program_error=$?
    set -e

    # Run gnuplot only if the program succeeded
    if [[ $program_error -eq 0 ]]; then
        set +e
        gnuplot $gnuplot_file
        gnuplot_error=$?
        set -e
    else
        rm -f running-zombie
        bad_parameter=1
        echo "Failed! Exit status: $program_error" >> "$log_file"
        return 0
    fi

    ...

    echo "Standard output: stdout-$1-$2-$3-$4-$5" >> "$log_file"
}

...
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

49

Now look at the **run_program** function in the **multi-sizes-errors** script, paying particular attention to the bits of the script highlighted above.

Can you work out what the highlighted bits are doing? Recall that the exit status of the last command that ran is stored in the special shell parameter **?**.

We observe that the logic of this function is that if the **zombie** program failed there's no point running **gnuplot** ("garbage in, garbage out"). We need to look a bit further down the function's definition (not shown above) to see what it does if **gnuplot** fails. Can you work out what it is doing (and why)?

If you are not sure, or you have any questions, please ask the course giver or a demonstrator.

You should try out this script and see what it does:

```
$ cd
$ rm -f *.dat *.png stdout-* logfile
$ cat scripts/bad_param_set | scripts/multi-sizes-errors
recovery (gamma) must be positive
Problem with parameter set: 1.0 -3.0 0.0005 50
recovery (gamma) must be positive
Problem with parameter set: 1.0 -3.0 0.0005 500
recovery (gamma) must be positive
Problem with parameter set: 1.0 -3.0 0.0005 5000
$ ls
```

The file **bad_param_set** contains one bad parameter set mixed in amongst some good ones, as you can see by inspecting it.

Version: Lent 2020

49

Nested ifs (1)

Do something only *if* some expression is true, **else** do another thing if another expression is true...and so on

```
if <command1> ; then
    <some commands>
elif <command2> ; then
    <some other commands>
elif <command3> ; then
    <yet other commands>
...
else
    <other commands>
fi
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

50

We can have even more complicated **if** statements than those we have met. We can *nest* **if** statements: if one command (or test) is true, do one thing, if a different command (or test) is true do something else and so on, culminating in an optional **else** section ("if none of the previous expressions were true, do this").

One of the easiest ways of doing this is by using **elif** (short for **else if**) for all the alternative expressions we want to test.

Why would we do this? Imagine that we had a shell script that could do several different things and the decision as to which it should do was made by the user specifying different arguments on the command line. We might want our script to have the following logic: if the user said "a" do this, else if they said "b" do that, else if they said "c" do something else, and so on, ending with else if they said something that was none of the previous things say "I don't know what you are talking about".

There are better ways to do that than using this sort of **if** statement, but they involve a construct (**case**) and a shell builtin command (**shift**) that we cover on the optional final day of this course.

50

Nested ifs (2)

```
#!/bin/bash

...

if [[ $1 = "one" ]] ; then
    first_function
elif [[ $1 = "two" ]] ; then
    second_function
elif [[ $1 = "three" ]] ; then
    third_function
elif [[ $1 = "four" ]] ; then
    fourth_function
else
    echo "Huh?" >&2
    exit 1
fi

$ cd
$ examples/nested-if one
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

51

In the `examples` subdirectory there is a silly shell script called `nested-if` that illustrates the nested `if` construct. The heart of the script is shown above – **`first_function`**, **`second_function`**, **`third_function`** and **`fourth_function`** are all shell functions defined in the script.

Try the script out and see what it does. Although it's a silly example, it should give you an idea of the sort of useful things for which you can use such scripts.

Second exercise



The `multi-sizes-errors` script is reasonably robust at dealing with bad parameter sets. However, it would be nice if it told us whether it was **`zombie`** or **`gnuplot`** which failed.

Modify this script so that in its `multi_sizes` function it prints different messages depending on whether it was **`gnuplot`** or **`zombie`** that failed. You may also need to modify other parts of the script as well.

When you've finished this exercise, take a short break (break = "not still in front of the computer") and then we'll look at the answer.

⏪ 10 minutes

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

52

The `multi-sizes-errors` shell script is in the `scripts` directory of your home directory. Your task is to modify this script – mainly the **`multi_sizes`** function – so that the **`multi_sizes`** function prints out different messages on standard error depending on whether it was **`zombie`** or **`gnuplot`** that failed. *Make sure you save your script after you've modified it.*

Some of you may be tempted to just dispense with `bash`'s "exit the shell script on any error" feature for this exercise. **Don't** – part of the purpose of this exercise is to get used to how the shell handles errors and how you work with this.

Remember that this shell script attempts to change directory – *a very dangerous thing to do in a shell script*, so you must make sure that if the script fails to change directory that it exits and doesn't try to do things in the wrong directory. The easiest way to do that is to have **`set -e`** in effect.

One approach that may occur to you is to make the function that runs **`zombie`** and **`gnuplot`** return different exit statuses depending on which of them failed. **Don't** do this – it fails in an extremely subtle way (which we'll look at later).

When you finish this exercise, take a short break and then we'll start again with the solution. (Yes, I really ***do*** mean "a break from the computer".)

Hint: One approach is to get the **`run_program`** function to set a shell variable to different values depending on whether it was **`zombie`** or **`gnuplot`** that failed. You could then test for this in the **`multi_sizes`** function.

Another hint: You may wish to use nested **`if`** statements, although they aren't the only way to do this exercise.

set -e revisited (1)

```
File: examples/function-exits
#!/bin/bash
set -e

function fail()
{
    # This function should always cause the script
    # to exit with a non-zero exit status
    echo "In function $FUNCNAME."
    set -e
    false
    echo "You should never see this message."
}

echo "About to run function fail."
fail
echo "Just ran function fail."

$ cd
$ examples/function-exits
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

53

In the `examples` subdirectory there is a shell script called `function-exits` which defines a function called **fail**. If we examine the function (shown on the slide above) we might hope that it would always trigger `bash`'s "exit the shell script on any error" feature (**set -e**). (Recall that **false** does nothing but returns a non-zero exit status, i.e. an error.)

Try the script out and see what it does...

(You should observe that the lines:

```
    echo "You should never see this message."
echo "Just ran function fail."
```

are never executed, and if you check the exit status of the shell script:

```
$ echo $?
```

you should observe it is non-zero: the shell script exited because the **false** command returned a non-zero exit status (i.e. it caused an "error").)

set -e revisited (2a)

```
File: examples/function-should-exit
#!/bin/bash
set -e

function fail()
{
    # This function should always cause the script
    # to exit with a non-zero exit status
    echo "In function $FUNCNAME."
    set -e
    false
    echo "You should never see this message."
}

echo "About to run function fail."
if fail ; then
    echo "Woo-hoo! Function fail succeeded."
else
    echo "Nooooo! Function fail didn't work."
fi

$ cd
$ cat examples/function-should-exit
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

54

Now look at the `function-should-exit` script in the `examples` subdirectory (shown on the slide above).

We might expect that, because we use **set -e** within the function **fail**, when we run that function it will cause the script to exit. But is this, in fact, the case?

Stop and think carefully about what messages you think this script would print on the screen if you ran it...

set -e revisited (2b)

Which of the following messages will you see if you run the function-should-exit script?:

1. In function fail.
2. You should never see this message.
3. About to run function fail.
4. Woo-hoo! Function fail succeeded.
5. Nooooo! Function fail didn't work.

```
$ cd
$ examples/function-should-exit
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

55

...and now run the `function-should-exit` script in the `examples` subdirectory and see which of the messages above it actually prints on the screen.

We might have expected that, because we use `set -e` within the function `fail`, when we run that function it will cause the script to exit. However, because we run the function as the command checked by an `if` statement, this doesn't happen! (We would have the same problem if we ran the function as the command checked by a `while` loop.)

Basically, if you run a shell function as the command checked by an `if` statement or a `while` loop, `set -e` is *disabled* whilst the function is running, even if you explicitly use it within the function. This makes using shell functions as the command checked by an `if` statement or a `while` loop extremely dangerous, so we advise you not to do it.

Give us Feedback!

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 Three

56

Final exercise

In your home directory is a program called **infect**, which is a simulation of the spread of infection in a closed population using a variant of the SIR model used in epidemiology. It prints its output (which are points on various graphs) to *standard output* and sends information about the parameters it has used to *standard error*. **infect** takes *three floating point* command line arguments and *one integer* command line argument. (It can also optionally take another three command line arguments (one floating point number, two integers) but we won't make use of those.)

In the **gnuplot** subdirectory there is a file of **gnuplot** commands called **infect.gnplt** that can be used to plot the data produced by **infect** – the commands in this file expect their input to be in a file called **infect.dat** in the current directory, and they produce a PNG file called **infect.png** (also in the current directory).

Write a shell script that will read the first three parameters for **infect** from standard input and the fourth parameter from the command line. It should run the **infect** program, turning its output into a graph using **gnuplot**. The following should illustrate how to combine the parameters from these two sources – suppose you read the following values from standard input:

```
1.0 0.1 0.0005 70
2.0 0.1 0.0005 250
```

...and the values **100 800** from the command line, then your script should run:

```
./infect 1.0 0.1 0.0005 100
./infect 1.0 0.1 0.0005 800
./infect 2.0 0.1 0.0005 100
./infect 2.0 0.1 0.0005 800
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

57

Please read this BEFORE you start on this exercise!

The point of this exercise is to consolidate everything you've learnt in this course thus far. To that end I want you to write your own shell script **FROM SCRATCH** to do this exercise – do *not* just take one of the ones we've constructed over this course and change the names of the programs it runs. Whilst you could certainly get an answer to this exercise that way, you wouldn't learn very much.

Also, I want your shell script to be *as good a shell script as you can possibly make it* – it should:

- be well structured using shell functions,
- be fully commented,
- do some error handling,
- keep a log file of what it is doing,
- print its error messages on standard error,
- use a temporary directory for working in,
- do some checking of its input,
- etc

There is a file in the **scripts** subdirectory called **infect_params** that you can use as a source of parameters to read via standard input. I suggest that for the command line arguments you use:

```
75 100 300 3000 50000
```

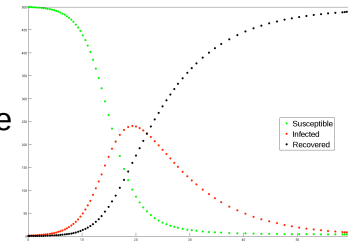
The files you need to do this exercise are available on-line at:

<https://help.uis.cam.ac.uk/help-support/training/downloads/course-files/programming-student-files/shellscripingsci/shellscripiting-files/exercises/day-three>

What is infect?

Simulation of the spread of infection in a closed population (a variant of the SIR model used in epidemiology)

green = Susceptible
red = Infected
black = Recovered



scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

58

For the curious: the **infect.py** program uses a variant of the SIR model to simulate the spread of an infection in a closed (i.e. no one enters or leaves) population. The SIR model is what is called a *compartmental* model in epidemiology. In such models the population is divided into a series of mutually exclusive categories (“compartments”). In the SIR model the categories are “Susceptible” (those susceptible to infection who have not yet caught it), “Infected” (those who have the infection) and “Recovered” (those who have recovered from the infection or who have natural immunity). (It is assumed that once you have recovered from the infection you can't be re-infected.)

The SIR model is a simple model that works well for modelling the spread of infectious diseases such as measles, mumps and rubella.

In the variant of the model used by the **infect.py** program, births and deaths have been added to the model (these are called “demographic events”), and the model is stochastic (i.e. events occur randomly according to how probable they are). However, so that it is easier to compare parameter sets, the default behaviour of the program is to use a fixed sequence of pseudo-random numbers, which means that given the same set of input parameters it should produce the same output.

The **infect.py** program writes its output to the screen as a collection of numbers rather than producing graphical output. If we capture that output to a file, we can then use that file to produce graphs of its output.

Running **infect** (1)

```
$ ./infect 1.0 0.1 0.0005 500
```

```
***
2.004760      172.000000      0.000000      314.000000
2.004760      172.000000      0.000000      313.000000
```

SIR model (including births and deaths) with [event-driven] demographic stochasticity

Population size: 5.0000e+02
Model run time: 2.0e+00 years

Initial number of susceptible individuals: 5.000e+01
Initial number of infected individuals: 3.000e+00

Transmission rate (beta): 1.000000e+00
Recovery rate (gamma): 1.000000e-01
Per capita birth [and death] rate (mu): 5.000000e-04

Model took 1.506090e-02 seconds

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

59

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

The **infect.py** program takes 4 numeric arguments on the command line: 3 positive floating-point numbers and 1 positive integer. It always writes its output to *standard output*, and also writes some informational messages to the *standard error*.

Running **infect** (2)

```
$ ./infect 1.0 0.1 0.0005 500 >infect.dat
```

SIR model (including births and deaths) with [event-driven] demographic stochasticity

Population size: 5.0000e+02
Model run time: 2.0e+00 years

Initial number of susceptible individuals: 5.000e+01
Initial number of infected individuals: 3.000e+00

Transmission rate (beta): 1.000000e+00
Recovery rate (gamma): 1.000000e-01
Per capita birth [and death] rate (mu): 5.000000e-04

Model took 1.506090e-02 seconds

As before, we have also provided a **gnuplot** script, in `gnuplot/infect.gplt`, that will produce graphs of the data output by **infect** if that data is in `infect.dat`.

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

60

The **infect.py** program sends its output to standard output, which we know how to capture to a file. Note that it also sends some information to *standard error* and this will not be captured by redirecting standard output to a file.

Running **infect** (3)

```
$ ./infect 1.0 0.1 0.0005 500 2>info
```

```
...
1.950702    169.000000    0.000000    316.000000
1.950702    170.000000    0.000000    316.000000
1.955447    170.000000    0.000000    316.000000
1.955447    171.000000    0.000000    316.000000
1.961349    171.000000    0.000000    316.000000
1.961349    170.000000    0.000000    316.000000
1.975273    170.000000    0.000000    316.000000
1.975273    170.000000    0.000000    315.000000
1.982251    170.000000    0.000000    315.000000
1.982251    171.000000    0.000000    315.000000
1.984463    171.000000    0.000000    315.000000
1.984463    171.000000    0.000000    314.000000
1.986952    171.000000    0.000000    314.000000
1.986952    172.000000    0.000000    314.000000
2.004760    172.000000    0.000000    314.000000
2.004760    172.000000    0.000000    313.000000
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

61

We can capture the messages that **infect** sends to standard error by redirecting standard error to a file. Note that this has no effect on what **infect** sends to standard output.

Running **infect** (4)

```
$ ./infect 1.0 0.1 0.0005 500 >infect.dat 2>info
```

```
$
```

We can control the format of the numbers in the informational messages with the environment variable **INFECT_FORMAT**:

```
$ INFECT_FORMAT=NORMAL ./infect 1.0 0.1 0.0005 500
```

```
...
2.004760    172.000000    0.000000    314.000000
2.004760    172.000000    0.000000    313.000000
```

SIR model (including births and deaths) with [event-driven] demographic stochasticity

Population size: 50

Model run time: 2.0 years

Initial number of susceptible individuals: 50

Initial number of infected individuals: 3

Transmission rate (beta): 1.0000

```
...
```

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

62

We can capture *both* standard output and standard error, to separate files, for **infect** as shown above: standard output will be redirected to the file **infect.dat** in the current directory and standard error will be redirected to the file **info** in the current directory.

Also, we can control the format of the numbers in the informational messages of the **infect** program using the **INFECT_FORMAT** environment variable. If we set the value of this variable to

NORMAL

then the numbers in the **infect** program's informational messages will *not* be in scientific notation (standard form).

Final exercise – Files



All the files (scripts, the **infect** and **zombie** programs, 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/
shellscripingsci/shells scripting-files/
exercises/day-three](https://help.uis.cam.ac.uk/help-support/training/downloads/course-files/programming-student-files/shellscripingsci/shells scripting-files/exercises/day-three)

If you are stuck for how to go about doing this exercise, have a look at the page after the next one for some ideas.

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している

Ta strona jest celowo pusta.

Esta página ha sido expresamente dejada en blanco.

Эта страница нарочно оставлена пустой.

Denne side med vilje efterladt tom.

Pağon intence vaka.

این صفحه خالی است

An leathanach seo fágtha folamh in aon turas.

This page intentionally left blank: nothing to see here. If you're stuck for how to go about doing the exercise, please see the next page.

Final exercise – Plan of action

What we want to do is:

1. Run **infect** with some parameters, capturing its output to `infect.dat`, and the messages it writes to standard error to `info-param1-param2-param3-param4`

```
$ INFECT_FORMAT=NORMAL ./infect 1.0 0.2 0.1 30  
>infect.dat 2>info-1.0-0.2-0.1-30
```
2. Run **gnuplot** with `infect.gplt` file

```
$ gnuplot infect.gplt
```
3. Rename created files (`infect.dat`, `infect.png`)

```
$ mv infect.dat infect-1.0-0.2-0.1-30.dat  
$ mv infect.png infect-1.0-0.2-0.1-30.png
```
4. Repeat the above steps for all the parameter sets...
5. Checking our input (where we can) to make sure it is sensible before running **infect**, and...
6. Handling errors properly.

scientific-computing@uis.cam.ac.uk

Simple Shell Scripting for Scientists: Day Three

65

Give us Feedback!

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 Three

66

So for this exercise you need to create a shell script that basically does the above task. When writing a shell script that is at all complicated, it is best to first plan it out, and one way of doing that is to describe what the shell script should do as a numbered list.

Basically, we want to run the **infect** program several times with a different parameter set each time, plotting its output on a graph each time. After each run, we rename the files we’ve created so that they don’t get overwritten.

Steps 1-3 can be straightforwardly achieved by writing a shell function that runs **infect**, then **gnuplot**, and then renames the files that have been created.

For step 4 we loop through the parameter sets. This is slightly more complicated than simply using a single loop since one of the parameters comes from standard input and the other from the command line. For step 5 we improve our shell script so that it checks its command line arguments. For step 6 we further improve our shell script to do some sensible error handling.