Introduction to Unix Shell Scripting

Day 2 - Building Blocks

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22-23 May 2024

Now that we understand shell operation, we can start discussing the main building blocks of a script.

- Parameters
 - Operations
- Control Statements
 - Conditionals
 - Loops
- ▶ Input and Output

Parameters I – setting and using simple parameters

Parameters

- A parameter (or variable) is just a name for a single value or a collection of values (known as an array).
- Scripts *store* values in variables for later use (often a transformation or decision).
- There are multiple ways of setting parameters, and many more ways of retrieving their values, including handy operations.
- ▶ We'll see about single-value parameters¹ now; arrays will be discussed later.

¹I'll just call them "simple" parameters.

Setting: the = operator

Assigns a value to a variable:

```
answer=42  # no need to declare (!= C...)
human='Homo sapiens' # quotes!
date=$(date); shell_msg="I use $SHELL"
species=$human  # no word splitting
answer="nuts!"  # can reassign freely
```

- There is **no whitespace** around the equals sign!
- Variable names (*identifiers*) contain **letters**, **digits**, **or underscores**; they cannot not start with a digit.
- \triangleright Expansions happen, but **word splitting is disabled**².

²Except for arrays - see below

Getting: \${}

Parameter expansion - retrieves the value of a variable.

```
place=Reykjavík # set value
echo ${place} # get value: ${...}
echo $place # short form
```

Unset and Null

- A *null* variable has the **empty string** ('') for a value.
- An *unset* variable **has no value** it does not exist (and it's usually a mistake to refer to its value³).
- A variable can be deleted with unset.

```
place=Bogotá
place='' # empty
place= # same as place=''
unset place # (NOT $place!) - deleted
```

³Think of NULL, null, nil, None, or Nothing in your favorite language.

Beware of the short form!

- Say we have files like <spc>_18S.dna, etc. for several species;
- Now we want to remove the files for some species, stored in variable \$spc.

```
spc=rat; rm $spc_18S.* # WRONG!
spc=rat; rm $spc_18S* # WORSE!! DON'T DO THIS!
spc=rat; rm ${spc}_18S* # correct
```

Can you guess what the rule is?

set -u guards against unset variables⁴.

⁴See Appendix I (day 2 slides).

Type

By default, Bash treats simple values as **strings**⁵. For Bash to treat a value as a number, it must usually be told to do so:

```
a=20; b=30; echo $a+$b  # surprise!
a=20; b=30; echo $((a+b)) # arithmetic
# malformed number -> 0
bond=oo7; echo $((bond))
```

⁵IOW, Bash is a (very) weakly-typed language.

String Operations I

```
genus=Harpagofututor
${#genus}  # length -> 14
${genus:7}  # substring from 7 (0-based)
${genus:0:7}  # substring of length 7 from 0
${genus: -5:4}  # SPACE is required (:-)
a=7; b=14
${genus:a:b}  # arithmetic evaluation
```

String Operations II

```
prog=BLASTN
${prog/N/P}
               # substitute 1st match
DNA=cgatgtattcag
RNA=${DNA//t/u}
                  # idem. all matches (t->u)
img=figure1.jpeg
${img%jp*g}svg
                  # delete pattern at end
ext=.png
$\{\img/.jp?g/\$ext\} # expansion happens
```

Many more variants (man bash).

Arithmetic Expansion: \$(())

Shell arithmetic: treats values as *integers*⁶ rather than strings:

- 1. Parameters are expanded (\$ not needed)
- 2. The resulting expression is evaluated numerically (operators on next slide)

```
a=2; b=5
echo $((a * b))
echo $((a < b)) # boolean - 1: true, 0: false</pre>
```

⁶As far as possible

Table 1: Main Arithmetic Operators, by decreasing precedence - () override.

operator	function
!	logical negation
**	exponentiation
*,/,%	multiplication, division, remainder
+, -	addition, subtraction
<, >, <=, >=	comparison
==, !=	logical equality and inequality
&&	logical AND
11	logical OR
=, +=, *=,	assignment

Simple Arithmetic Tests: (())⁸

- This is a *command*. It succeeds if the arithmetic expression between ((and)) result is **not** zero.
- ➤ Combined with && and/or ||, provides *simple*⁷ decision making.

```
((N < 10)) && echo "sample too small"
((N < 10)) && echo "too small" || echo "large enough"
# ==, !=, <= ...
```

⁷There are other, more flexible forms.

⁸Not the same as \$(()) (arithmetic expansion)

Why can 0 signal both success and failure?

Historical aside

- Unix: (many) more ways to fail than to succeed \rightarrow 0 for success, > 0 for various kinds of errors.
- ► Early shells: crude Boolean and arithmetic expressions (if at all).
- C language: Boolean algebra with 0 for false and nonzero for true.
- \Rightarrow When (or "if") arithmetic and Boolean expressions were added to shells, they were strongly influenced by C.^a

^aAs was the for ((;;)) loop.

Simple Tests involving String Values: [[]]

Like (()), but with strings.

- ► [[]] is a command, and succeeds IFF the *conditional expression* within it evaluates to true.
- ightharpoonup It can also be combined with &&, ||, etc.

```
[[ $s ]] # $s is non-empty
[[ $s = $t ]] # $s is the same (string) as $t
```

- Spaces matter
- ➤ Word splitting is **disabled** between [[]], so "\$var" can be simplified to \$var

⁹Like any command, in fact

More String Comparison

<, >, etc. also available, but with some differences:

```
[[ Amanda > Pam ]] # Lexical -> false
[[ 2+2 == 4 ]] # false!
[[ 10 < 2 ]] # true!</pre>
```

[[...]] *can* compare numbers 10

¹⁰Though perhaps it shouldn't be used for that.

File Properties

They take the form -c filename, where the character c denotes a file property. For example, to check if a file exists, use -e:

```
[[ -e file.txt ]] && echo "exists!"
# Make a dir unless it exists
[[ -d mydir ]] || mkdir mydir
```

Many properties can be tested in this way (see next slide).

Other file property test operators

operator	true if
-f	file exists and is a regular file (e.g., not a dir)
-r	file is readable
-w	file is writable
-x	file is executable
-s	file exists and has a size greater than 0

There are also a few file *comparison* operators, such as f1 -nt f2 which is true iff f1 is newer than f2. Obviously, they expect *two* arguments.

Pattern Matching

If unquoted, the right-hand argument of a == or != is treated as a pattern ("glob"):

```
[[ abc == ?bc ]] # true
[[ abc == "?bc" ]] # false (quotes)
gene=lacZ; [[ $gene == lac? ]]
```

Note that the glob pattern isn't matched against files, but against the **left-hand argument**.

It is also possible to match against regular expressions (see supplementary slides).

Expansion Happens

The above examples used mostly literals for simplicity's sake, but (most) expansions are entirely possible in test commands:

```
[[ -x $HOME ]] # better not be false
[[ $SHELL == /usr/bin/bash ]]
[[ /usr/bin/echo == $(which echo) ]]
a=1; b=1; [[ $a -eq $b ]]
(($(ls | wc -l) > 10)) && echo 'more than ten files'
```

Logical Operations

The expressions can be connected with the logical operators (...), !, &&, and || (decreasing order of precedence).¹¹

```
a=Ann; b=Ben; [[ $a == $a && ! ($b == $b) ]]
# Also works with (( ))
a=2; b=3; ((a != b || a == b))
```

¹¹The *logical* operators &&, ||and! are **not the same** as the *control* operators &&, ||and!.

Practice

 \rightarrow Exercise 2.1

I/O - Getting data into and out of our script

Input

There are many ways of getting data into our script, including:

- Reusing standard input
- Positional parameters
- The read and mapfile functions
- Command substitution: \$(...)
- Environment variables

Standard Input (stdin)

Commands called by a script inherit its standard input:

```
#!/bin/bash
# reuse_stdin.sh
grep Spo0
# at this point, stdin is used up!
```

```
./reuse_stdin.sh < ../data/SpoOA.msa
```

grep's stdin is the same as reuse_stdin.sh's, namely
../data/Spo0A.msa.

Practice

 \rightarrow **Exercise 2.2** - Reusing standard input.

Arguments and Positional Parameters

A command's arguments are accessed through special parameters called *positional parameters*: **\$1**, **\$2**, etc., which hold the first, second, etc. arguments, respectively.

./show_args.sh -f -y optarg arg1 arg{2..4}

- \$0 holds the name of the script (or function).
- ▶ \$@ holds all argument values passed to the script (or function).
- > \$# holds the count of the number of argument values passed to the script (or function).

We can now change our script to:

```
#!/bin/bash
# pos_arg.sh
grep Spo0A "$1"
```

```
./pos_arg.sh ../data/SpoOA.msa
```

Sadly, the script now longer works with the < redirection, because then there is no \$1 (do set -u to check). ¹²

¹²But there is a way to make a script work in both ways.

Reading by lines - read

Instead of reading whole files, as we did up to now...

... the read builtin¹³ takes one or more identifiers, reads one line, word-splits it, and sets the corresponding identifiers:

```
read firstname lastname echo "Hi, $firstname $lastname!"
```

 $^{^{13}\}mathrm{A}$ builtin command works like a program but is part of the shell

Practice

 \rightarrow **Exercise 2.3** - Getting user input from arguments.

Environment Variables: export

```
#!/bin/bash
printf "NOT_EXPORTED: %s\n" "$NOT_EXPORTED"
printf " EXPORTED: %s\n" "$EXPORTED"
```

Try the following:

```
unset EXPORTED NOT_EXPORTED
NOT_EXPORTED='not exported'
export EXPORTED=exported  # inherited
./use_env.sh
```

Use case: HPC clusters (can't pass parameters).

Output

- echo: just outputs its arguments, separated by spaces. By default, doesn't handle $\ensuremath{\mbox{-escapes}^{14}}$. Terminates lines with a \n unless told not to (-n).
- printf: formatted printing (see below); \t and \n work as expected.
- Any programs called will use our script's stdout and stderr.

¹⁴Compare echo 'a\tb' and echo -e 'a\tb'.

printf¹⁵ - formatted printing

- Takes a *format string* and zero or more further arguments.
- ▶ *Placeholders* in the format string are replaced by the corresponding arguments (in order).
- Formats allow control over length, decimal places, padding, etc.

¹⁵Inherited from the C language, and copied by countless others.

printf - Examples

```
pi=3.1415926535; seq=CAGCACACCG;
printf "The value of Pi is about %.2f\n" "$pi"
printf "First 5 residues of seq: %.5s\n" "$seq"
printf "%02d\n" {1..10} # handy for sorting
```

- %f treats the argument as a floating-point value.
- %s treats the argument as a string.
- %d treats the argument as an integer.
- \rightarrow use echo for simple tasks, printf for anything else.

Control Structures

Only the simplest scripts run all their code exactly once. Most execute at least *some* instructions more than once, or not at all.

For this, we use *control structures*:

- Loops (repetition) shortly
- Conditionals (choice) later
- Groups (sequential flow) not covered

They start and stop with a specific **keyword** (if...fi, {...}, while...done, etc.)

Test Commands

As we will see shortly, many conditionals and loops involve *test commands*. They are typically one of the following (all already known!):

- a simple command the test succeeds iff the command succeeds (returns 0);
- a conditional expression between [[and]]
- **an** arithmetic expression between ((and))

Loops

Loops are **iterative** control structures: they **repeat** a sequence of commands (called the *body*), typically with minor modifications.

They operate either:

- For a **fixed** number of iterations (for ... in). No test command is involved in this form.
- Until some **condition** is met (while, until, for ((...))). This condition is expressed as a test command.

for loop - 1st form

Expands <words>, and executes <commands>, binding <name> to each of the resulting values in turn.

Sometimes written with more (or fewer); instead of newlines.

The second form of the for loop allows e.g. a dummy variable – see supplementary slides.

for loop - Example 1

for loops are frequently used with file globs. The following copies a set of *.fasta files to *.fas:

```
for file in *.fasta ; do
  cp $file ${file/.fasta/.fas}
done
```

while loop

In while loops, the body is executed **as long as <test> succeeds**.

```
while <test> ; do
    <commands> # body
done
```

(The similar until loop works in the same way, except that it loops **until** the test succeeds (see Supplementary slides)).

Example: the Collatz conjecture

```
#!/usr/bin/env bash
declare -i n=$1
while ((n > 1)); do
    printf "%d\n" "$n"
    if ((0 == n \% 2)); then
         ((n /= 2))
    else
         ((n = 3*n +1))
    fi
done
```

Skipping iterations - the continue keyword

All loops (for, while, and until) support the use of the continue keyword, that makes execution of code skip the remainder of the current loop.

Example: print all multiples of 7 between 0 and 100.

```
for x in {0..100}; do
   ((x % 7 != 0)) && continue
   echo $x
done
```

Breaking out of Loops - the break keyword

break allows an early exit from a loop:

```
# Print the first line that contains some string.
while read line; do
  if [[ $line == *GAATTC* ]]; then
    printf "%s\n" "$line"
    break
  fi
done
```

To break out of n nested loops, use break n.

Practice

 \rightarrow **Exercise 2.4** - a simple for loop.

Conditionals

Conditionals are *branching* control structures. They enable the script to **choose what to do** between two or more possibilities.

The main conditional constructs are:

- if yes-or-no decisions (possibly nested), based on a *test* command
- case multi-way decision, based on pattern matching

if

The basic idea:

```
if <test-command> ; then
    <statements> # iff test-command returns 0
fi
```

See check_user.sh for an example.

Before we look in detail at test commands, we need to see the full version:

- There can be 0 or more elif clauses.
- There can be 0 or 1 else clause.

Parameters II - Arrays

Arrays: Collections

While a simple parameter stores a single value, an array is a **collection**: it can store more than one value.

Kinds of Arrays

- indexed arrays¹⁶ store lists of values referred to by a nonnegative integer, e.g. lines [3], lines [4] and lines [10] could contain some lines from a file;
- associative arrays store key-value pairs, e.g. nb_reads['rec_A'] for the number of reads mapping to the recA gene, nb_reads['ox1T'] the number mapping to oxlT, etc.

We will cover indexed arrays, see the supplementary slides for the associative variety.

¹⁶or just "arrays" for short

Indexed Arrays

Accessing All Array Elements

Using * or @ as index refers to all array elements, but with subtle differences depending on quoting:¹⁷

```
names=('Bilbo Baggins' Beorn Gollum)
showa ${names[@]} # (or *): 4 arguments!
showa "${names[@]}" # 3 arguments
showa "${names[*]}" # 1 argument
IFS=','; echo "${names[*]}"; unset IFS
```

The # operator yields the number of elements

```
echo ${#names[@]} # (or *)
```

¹⁷And also on whether or not word splitting occurs.

Iterating over an Array

```
for e in "${array[@]}"; do ... ; done
```

Example of Array Usage

Cf. ../src/pascal.sh

Arrays and Word Splitting

Word splitting is *NOT disabled* when creating arrays:

```
elements='A B "C D"' # no split
array=($elements) # split -> 4 elements!
```

Neither is file globbing:

```
pdf_glob=*.pdf; echo "$pdf_glob"
PDF_S=$pdf_glob; echo "$PDF_S"
PDF_A=($pdf_glob); declare -p PDF_A
```

Array Caveats

▶ If no index is given, 0 is assumed:

Arrays can't be assigned as values:

```
# Try to make a copy of `names`
lotr_names=names # WRONG - string assignment
lotr_names=$names # WRONG - see above
lotr_names=(${lotr_names[@]}) # OK
```

Functions

Motivating Example

See ./src/func_motiv*.sh

Functions

A *function* is like a miniature script that can be called from within another script. Calling a function causes its code to be executed, but does not by itself start a new process.

We write functions in order to:

- Re-use code (DRY principle).
- Improve the clarity of the code.
- Avoid creating new processes (they have a cost: see noop_test.sh)

Definition

Functions are defined with one of the following forms:

Call

A function is called just like a command. Arguments are passed in the same way:

```
my_func arg1 "$value"
```

Positional parameters (\$1, \$0, shift, etc.) work in the same way as in scripts.

Local Variables

By default, all variables in Bash are **global**: once set, they can be accessed from anywhere in the script.

Variables defined in a function can¹⁸ be declared as **local**, so that they are only available in the namespace of that function:

```
my_var='a'
my_func() {
  local my_var='b' # A different variable.
}
```

See ../src/func.sh.

¹⁸And usually should

"Returning values" from functions

Shell functions **do not** return values¹⁹: instead, they return an exit status, again behaving like commands.

To pass data back to the caller: (i) have the function output the value of interest, and (ii) use command substitution over the function call.

```
my_func() { echo "Hi!"; }
result=$(my_func) # Called just like any command.
```

The exit status is that of the last command in the function body, but it can be overridden with the return keyword.

¹⁹Unlike in pretty much every other language.

Practice

Let's practice using functions to avoid duplication.

 \rightarrow **Exercise 2.5** - Introduction to functions.

Conclusion

- We have seen how the shell operates, including tokenizing, parsing, the various forms of expansions, conditionals and arithmetic.
- ▶ We have used this knowledge (and more) to write a script that converts Fasta to CSV. It's not efficient, but it's easy to understand.
- You should now be able to start writing your own scripts.

May You Solve Interesting Problems

For some people, myself included, the satisfaction of solving a problem is the difference between work and drudgery. [...] Besides, once I accomplish my task, I congratulate myself on being clever. I feel like I have done a little bit of magic and spared myself some dull labor.

Dale Dougherty and Arnold Robbins, sed & awk (2010)

Learning shell scripting - Resources

- man bash always handy, if a bit terse.
- help for Bash builtins etc.
- ► The Bash website and especially the Bash Manual (not the same as man bash!).
- ► The Advanced Bash Scripting Guide.
- ► The Bash Cheat Sheet.
- ▶ The Bash Programming Reference. is another cheatsheet, more specialized towards programming.

- ► Shellcheck static analysis tool
- ► Bash Cookbook
- ► Bash Idioms

Thanks!

- Thank you all for your attention!
- Special thanks to Robin
- ▶ Thanks to the Course Organizers

Supplementary Slides

Arguments don't have to be filenames

- We have used \$1 to specify a data file (by its name).
- The effect is similar to redirecting stdin to that file.
- This is very frequent.
- But positional parameters can of course used for countless other purposes.

read (cont'd)

The command fails (returns 1) if it can't read anything.

There can be more than one identifiers:

```
read x y z <<< '1 2 3'
# x=1, y=2, y=3
```

read (final)

If there are more words (after splitting) than there are identifiers, the last identifier gets the extra words:

```
read x y z <<< '1 2 3 4 5'
# x: 1, y: 2, z: 3 4 5
```

If there is only one identifier, it captures the whole line:

read line

If there are fewer words than identifiers, the extra identifiers are set to an empty string.

for loop - Example 2

Another typical case is with a sequence, often generated by a brace expansion (here $\{1..10\}$ expands to the numbers from 1 to 10):

```
# Compute the squares of numbers from 1 to 10. for n in \{1..10\}; do echo \$((n**2)); done
```

(recall that \$((...)) is arithmetic expansion)

for loop - 2nd form ("C form")

Another way to write a for loop is using the \mathbf{C} syntax 20 .

```
for ((<start-cmd>; <condition>; <iteration-cmd>)); do
      list>;
done
```

- 1. Evaluate <start-cmd>.
- 2. Evaluate <condition>; if true execute <list>, if not exit loop.
- 3. Evaluate <iteration-cmd> and go back to 2.

The evaluations are done in shell arithmetic.

²⁰So named because it was copied from the C language

Example: for loop, 2nd form

```
# Powers of 2 smaller than 10000.
for ((p=1; p<10000; p=2*p)); do
   echo $p
done</pre>
```

Notes:

- Geometric, not arithmetic progression (as in {1..10}).
- Only numeric (no globs, etc.).

until loop

This works like the while loop, except that the body is executed as long as the test *fails*.

```
until <conditional> ; do
  <statements>
done
```

Constants

You can prevent a parameter from changing values

```
declare -r PI=3.14159
PI=4096
# -> bash: PI: readonly variable
```

Readonly variables can't be unset.

Defaults for Null and Unset

The "default" operator : - substitutes a value if a parameter is unset or null.

```
unset notset
echo $notset
echo ${notset:-default}
null=
echo $null
echo ${null:-default}
```

Variants

- = also *sets* the variable.
- ▶ Both have forms (-, =) that only check for unset (not null).

Notes:

- ► There must be **no whitespace** around -, :-, etc..
- ► The right-hand side is *expanded*:

```
unset var; msg="Unset var!"; echo ${var-$msg}
```

Associative Arrays

Associative arrays *must* be declared as such:

```
declare -A aar
aar[key1]=val1
declare -A aar=(K1 V1 K2 V2)
echo ${aar[key1]}
```

The behaviour is otherwise very similar to that of indexed arrays.

Note: * and @ work on the *values*, to expand the *keys* use a !: \${!aar[*]}, etc.

Associative Array Caveats

The order in which associative array elements are expanded is **unpredictable**. In particular, there is *no guarantee* that values (or keys) will be listed in the order they were added to the array.

Matching Regular Expressions

The =~ operator matches against POSIX regular expressions²¹

```
[[ abc =~ .bc ]] # true
[[ abc =~ abc? ]] # true
[[ abc == abc? ]] # false (glob)
```

²¹à la grep, Perl, sed, and so many others... each with its own dialect, all different from globs:-(

No floating-point?

```
echo $((5/2)) # wtf?
echo $((5.0/2.0)) # fails!
```

 \rightarrow use an external program²²

```
echo "scale=1; $b/$a" | bc
bc <<< "$scale=1; $b/$a"
result=$(bc <<< "$scale=1; $b/$a") && echo $result
```

²²In the same way you use sed, awk etc. when the shell's string functions are too limited

String Conditionals

The following operate on strings

Operator	True if
s	s is a non-empty string
s1 == s2	s1 and s2 are equal strings
s1 = s2	idem (note spaces!)
s1 != s2	s1 and s2 are different
s1 < s2	s1 comes before s2 alphabetically
s1 > s2	s1 comes after s2 alphabetically

Numeric Conditionals

The following operators also operate on strings, but *treat their operands numerically*²³:

Operator	Meaning (numerically)
<u>- F</u>	
s1 -eq s2	s1 = s2
s1 -ne s2	$\mathrm{s}1 \neq \mathrm{s}2$
s1 -lt s2	s1 < s2
s1 -le s2	$s1 \le s2$
s1 -gt s2	s1 > s2
s1 -ge s2	$s1 \ge s2$

²³Using shell arithmetic, more on this shortly

This way things make more sense:

```
[[ 2+2 -eq 4 ]] # true
[[ 10 -lt 2 ]] # false!
```

Appendix I: Sample Formats

General Feature Format (GFF)

```
##gff-version 3.1.26
##sequence-region ctg123 1 1497228
ctg123 . gene 1000 9000 . + . ID=gene00001; Name=EDEN
ctg123 . mRNA 1050 9000 . + . ID=mRNA00001; Parent=...
ctg123 . mRNA 1050 9000 . + . ID=mRNA00002; Parent=...
ctg123 . mRNA 1300 9000 . + . ID=mRNA00003; Parent=...
ctg123 . exon 1300 1500 . + . ID=exon00001; Parent=...
ctg123 . exon 1050 1500 . + . ID=exon00002; Parent=...
ctg123 . exon 3000 3902 . + . ID=exon00003; Parent=...
```

Variant Call Format (VCF)

```
##fileformat=VCFv4.3
##source=myImputationProgramV3.1
#CHR.OM
        POS
                TD
                                        QUAL
                                                     INFO
                            REF
                                T.TA
                                             FILTER
20
                rs6054257
                                        29
                                             PASS
                                                     NS=3:.
        14370
                                Α
20
        17330
                                        3
                                             q10
                                                     NS=3:.
20
        1110696 rs6040355 A
                                G,T
                                        67
                                             PASS
                                                     NS=2:
20
        1230237
                                        47
                                             PASS
                                                     NS=3:.
20
        1234567 microsat1 GTC G.GTCT 50
                                             PASS
                                                     NS=3:.
```