



Shell Scripting

Alexander B. Pacheco
LTS Research Computing

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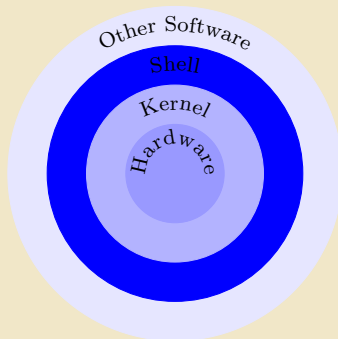
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Introduction

What is a SHELL

- The command line interface is the primary interface to Linux/Unix operating systems.
- Shells are how command-line interfaces are implemented in Linux/Unix.
- Each shell has varying capabilities and features and the user should choose the shell that best suits their needs.
- The shell is simply an application running on top of the kernel and provides a powerful interface to the system.



Types of Shell

sh : Bourne Shell

- ◆ Developed by Stephen Bourne at AT&T Bell Labs

csh : C Shell

- ◆ Developed by Bill Joy at University of California, Berkeley

ksh : Korn Shell

- ◆ Developed by David Korn at AT&T Bell Labs
- ◆ backward-compatible with the Bourne shell and includes many features of the C shell

bash : Bourne Again Shell

- ◆ Developed by Brian Fox for the GNU Project as a free software replacement for the Bourne shell (sh).
- ◆ Default Shell on Linux and Mac OSX
- ◆ The name is also descriptive of what it did, bashing together the features of sh, csh and ksh

tcsh : TENEX C Shell

- ◆ Developed by Ken Greer at Carnegie Mellon University
- ◆ It is essentially the C shell with programmable command line completion, command-line editing, and a few other features.

Shell Comparison

	sh	csH	ksh	bash	tcsh
Programming Language	✓	✓	✓	✓	✓
Shell Variables	✓	✓	✓	✓	✓
Command alias	✗	✓	✓	✓	✓
Command history	✗	✓	✓	✓	✓
Filename completion	✗	★	★	✓	✓
Command line editing	✗	✗	★	✓	✓
Job control	✗	✓	✓	✓	✓

✓ : Yes

✗ : No

★ : Yes, not set by default

<http://www.cis.rit.edu/class/simg211/unixintro/Shell.html>

Variables I

- A variable is a named object that contains data used by one or more applications.
- There are two types of variables, Environment and User Defined and can contain a number, character or a string of characters.
- Environment Variables provides a simple way to share configuration settings between multiple applications and processes in Linux.
- As in programming languages like C, C++ and Fortran, defining your own variables makes the program or script extensible by you or a third party
- Rules for Variable Names
 - ❶ Variable names must start with a letter or underscore
 - ❷ Number can be used anywhere else
 - ❸ DO NOT USE special characters such as @, #, %, \$
 - ❹ Case sensitive
 - ❺ Examples
 - Allowed: VARIABLE, VAR1234able, var_name, _VAR
 - Not Allowed: 1VARIABLE, %NAME, \$myvar, VAR@NAME
- To reference a variable, environment or user defined, you need to prepend the variable name with "\$" as in \$VARIABLE, \$PATH, etc.

Variables II

- Its a good practice to protect your variable name within `{...}` such as `${PATH}` when referencing it. (We'll see an example in a few slides)
- Assigning value to a variable

Type	sh,ksh,bash	csh,tcsh
Shell	name=value	set name = value
Environment	export name=value	setenv name value

- **sh,ksh,bash** THERE IS NO SPACE ON EITHER SIDE OF =
- **csh,tcsh** space on either side of = is allowed for the **set** command
- **csh,tcsh** There is no = in the **setenv** command

File Permissions I

- In *NIX OS's, you have three types of file permissions
 - 1 read (r)
 - 2 write (w)
 - 3 execute (x)
- for three types of users
 - 1 user
 - 2 group
 - 3 world i.e. everyone else who has access to the system

drwxr-xr-x.	2	user	user	4096	Jan	28	08:27	Public
-rw-rw-r--.	1	user	user	3047	Jan	28	09:34	README

- The first character signifies the type of the file
 - d for directory
 - l for symbolic link
 - for normal file
- The next three characters of first triad signifies what the owner can do
- The second triad signifies what group member can do

File Permissions II

- The third triad signifies what everyone else can do

$$\begin{array}{c} \text{g} \\ \text{d} \text{rwx} \text{r} - \text{x} \text{r} - \text{x} \\ \text{u} \qquad \qquad \text{o} \end{array}$$

- Read carries a weight of 4
- Write carries a weight of 2
- Execute carries a weight of 1
- The weights are added to give a value of 7 (rwx), 6(rw), 5(rx) or 3(wx) permissions.
- `chmod` is a *NIX command to change permissions on a file
- To give user rwx, group rx and world x permission, the command is

```
chmod 751 filename
```

- Instead of using numerical permissions you can also use symbolic mode

u/g/o or a user/group/world or all i.e. ugo

+/- Add/remove permission

r/w/x read/write/execute

File Permissions III

- Give everyone execute permission:

```
chmod a+x hello.sh
```

```
chmod ugo+x hello.sh
```

- Remove group and world read & write permission:

```
chmod go-rw hello.sh
```

- Use the **-R** flag to change permissions recursively, all files and directories and their contents.

```
chmod -R 755 ${HOME}/*
```

What is the permission on `${HOME}`?

HPC Users

If you want to share your files with your colleagues

- 1 Make your home directory read accessible to the world

```
chmod 755 ${HOME}
```

DO NOT USE THE RECURSIVE **-R** FLAG


- 2 Change to your home directory and give read access to the directory that you want to share using the **-R** flag

Input/Output I


- For reading input from screen/keyboard/prompt

bash `read`

tcsh `$<`

- The `read` statement takes all characters typed until the  key is pressed and stores them into a variable.

Syntax `read <variable name>`

Example `read name` 

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- `$<` can accept only one argument. If you have multiple arguments, enclose the `$<` within quotes e.g. `"$<"`

Syntax: `set <variable> = $<`

Example: `set name = "$<"` 

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- In the above examples, the name that you enter is stored in the variable `name`.

Input/Output II

- The command `echo` is used for displaying output to screen
- Use the `echo` command to print the variable `name` to the screen

```
echo $name 
```

- The `echo` statement can print multiple arguments.
- By default, `echo` eliminates redundant whitespace (multiple spaces and tabs) and replaces it with a single whitespace between arguments.
- To include redundant whitespace, enclose the arguments within double quotes

```
echo Welcome to HPC    Training← (more than one space between HPC and Training)
```

```
echo "Welcome to HPC    Training"←
```

```
read name← or set name = "$<"←
```

```
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```

```
echo $name←
```

```
echo "$name"←
```

Input/Output III

- You can also use the **printf** command to display output

Syntax: `printf <format> <arguments>`

Example: `printf "$name"←`

`printf "%s\n" "$name"←`

- Format Descriptors

`%s` print argument as a string

`%d` print argument as an integer

`%f` print argument as a floating point number

`\n` print new line

you can add a width for the argument between the `%` and `{s,d,f}` fields

`%4s`, `%5d`, `%7.4f`

- The **printf** command is used in **awk** to print formatted data (more on this later)

I/O Redirection

- There are three file descriptors for I/O streams
 - ① STDIN: Standard Input
 - ② STDOUT: Standard Output
 - ③ STDERR: Standard Error
- 1 represents STDOUT and 2 represents STDERR
- I/O redirection allows users to connect applications
 - < : connects a file to STDIN of an application
 - > : connects STDOUT of an application to a file
 - >> : connects STDOUT of an application by appending to a file
 - | : connects the STDOUT of an application to STDIN of another application.
- Examples:
 - ① write STDOUT to file: `ls -l > ls-l.out`
 - ② write STDERR to file: `ls -l 2> ls-l.err`
 - ③ write STDOUT to STDERR: `ls -l 1>&2`
 - ④ write STDERR to STDOUT: `ls -l 2>&1`
 - ⑤ send STDOUT as STDIN: `ls -l | wc -l`

Shell Scripting

What is a scripting language?

- A **scripting language** or **script language** is a *programming language* that supports the writing of **scripts**.
- **Scripting Languages** provide a higher level of abstraction than standard programming languages.
- Compared to programming languages, scripting languages do not distinguish between data types: integers, real values, strings, etc.
- Scripting Languages tend to be good for automating the execution of other programs.
 - ◆ analyzing data
 - ◆ running daily backups
- They are also good for writing a program that is going to be used only once and then discarded.
- A **script** is a program written for a software environment that automate the execution of tasks which could alternatively be executed one-by-one by a human operator.
- The majority of script programs are “quick and dirty”, where the main goal is to get the program written quickly.

Writing your first script

Three things to do to write and execute a script

1 Write a script

- A shell script is a file that contains ASCII text.
- Create a file, `hello.sh` with the following lines

```
#!/bin/bash
# My First Script
echo "Hello World!"
```

2 Set permissions

```
~/Tutorials/BASH/scripts> chmod 755 hello.sh
```

OR

```
~/Tutorials/BASH/scripts> chmod a+x hello.sh
```

3 Execute the script

```
~/Tutorials/BASH/scripts> ./hello.sh
Hello World!
```

4 If you do not set execute permission for the script, then

```
~/Tutorials/BASH/scripts> sh hello.sh
Hello World!
```

Description of the script

- My First Script

```
#!/bin/bash
# My First Script
echo "Hello World!"
```

- The first line is called the "ShaBang" line. It tells the OS which interpreter to use. In the current example, bash
- Other options are:
 - ◆ sh : #!/bin/sh
 - ◆ ksh : #!/bin/ksh
 - ◆ csh : #!/bin/csh
 - ◆ tcsh: #!/bin/tcsh
- The second line is a comment. All comments begin with "#".
- The third line tells the OS to print "Hello World!" to the screen.

Special Characters

`#`: starts a comment.

`$`: indicates the name of a variable.

`\`: escape character to display next character literally.

`{ }`: used to enclose name of variable.

`;` Command separator [semicolon]. Permits putting two or more commands on the same line.

`;;` Terminator in a case option [double semicolon].

`.` "dot" command [period]. Equivalent to source. This is a bash builtin.

`$?` exit status variable.

`$$` process ID variable.

`[]` test expression

`[[]]` test expression, more flexible than `[]`

`$[]`, `(())` integer expansion

`||`, `&&`, `!` Logical OR, AND and NOT

Quotation

- Double Quotation " "
- Enclosed string is expanded ("\$", "/" and "")
- Example: `echo "$myvar"` prints the value of `myvar`
- Single Quotation ' '
- Enclosed string is read literally
- Example: `echo '$myvar'` prints `$myvar`
- Back Quotation ` `
- Used for command substitution
- Enclosed string is executed as a command
- Example: `echo `pwd`` prints the output of the `pwd` command i.e. print working directory
- In **bash**, you can also use `$(...)` instead of ``...``
e.g. `$(pwd)` and ``pwd`` are the same

Example

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

```
HI=Hello
```

```
echo HI           # displays HI
echo $HI          # displays Hello
echo \ $HI        # displays $HI
echo "$HI"        # displays Hello
echo '$HI'        # displays $HI
echo "$HIAlex"    # displays nothing
echo "${HI}Alex"  # displays HelloAlex
echo `pwd`        # displays working directory
echo $(pwd)       # displays working directory
```

```
~/Tutorials/BASH/scripts/day1/examples> ./quotes.sh
HI
Hello
$HI
Hello
$HI

HelloAlex
/home/apachecco/Tutorials/BASH/scripts/day1/examples
/home/apachecco/Tutorials/BASH/scripts/day1/examples
~/Tutorials/BASH/scripts/day1/examples>
```

Arithmetic Operations I

- You can carry out numeric operations on integer variables

Operation	Operator
Addition	+
Subtraction	-
Multiplication	*
Division	/
Exponentiation	** (bash only)
Modulo	%

- Arithmetic operations in **bash** can be done within the `$((...))` or `#[...]` commands
 - ★ Add two numbers: `$((1+2))`
 - ★ Multiply two numbers: `#[a*b]`
 - ★ You can also use the `let` command: `let c=a-b`
 - ★ or use the `expr` command: `c='expr a - b'`

Arithmetic Operations II

- In **tcsh**,

- ★ Add two numbers: `@ x = 1 + 2`
- ★ Divide two numbers: `@ x = $a / $b`
- ★ You can also use the **expr** command: `set c = `expr $a % $b``

- Note the use of space

bash space required around operator in the **expr** command

tcsh space required between `@` and variable, around `=` and numeric operators.

- You can also use C-style increment operators

bash `let c+=1` or `let c--`

tcsh `@ x -= 1` or `@ x++`

`/=`, `*=` and `%=` are also allowed.

bash

- The above examples only work for integers.
- What about floating point number?

Arithmetic Operations III

- Using floating point in **bash** or **tcsh** scripts requires an external calculator like GNU **bc**.
 - ★ Add two numbers:
`echo "3.8 + 4.2" | bc`
 - ★ Divide two numbers and print result with a precision of 5 digits:
`echo "scale=5; 2/5" | bc`
 - ★ Call **bc** directly:
`bc <<< "scale=5; 2/5"`
 - ★ Use **bc -l** to see result in floating point at max scale:
`bc -l <<< "2/5"`
- You can also use **awk** for floating point arithmetic.

Flow Control

- Shell Scripting Languages execute commands in sequence similar to programming languages such as C, Fortran, etc.
- Control constructs can change the sequential order of commands.
- Control constructs available in **bash** and **tcsh** are
 - ① Conditionals: `if`
 - ② Loops: `for`, `while`, `until`
 - ③ Switches: `case`, `switch`

if statement

- An **if/then** construct tests whether the exit status of a list of commands is 0, and if so, executes one or more commands.

bash

```
if [ condition1 ]; then
    some commands
elif [ condition2 ]; then
    some commands
else
    some commands
fi
```

tcsh

```
if ( condition1 ) then
    some commands
else if ( condition2 ) then
    some commands
else
    some commands
endif
```

- Note the space between *condition* and "[" "]"
- **bash** is very strict about spaces.
- **tcsh** commands are not so strict about spaces.
- **tcsh** uses the **if-then-else if-else-endif** similar to Fortran.

Comparison Operators

Integer Comparison		
Operation	bash	tcsh
equal to	if [1 -eq 2]	if (1 == 2)
not equal to	if [\$a -ne \$b]	if (\$a != \$b)
greater than	if [\$a -gt \$b]	if (\$a > \$b)
greater than or equal to	if [1 -ge \$b]	if (1 >= \$b)
less than	if [\$a -lt 2]	if (\$a < 2)
less than or equal to	if [\$a -le \$b]	if (\$a <= \$b)

String Comparison		
operation	bash	tcsh
equal to	if [\$a == \$b]	if (\$a == \$b)
not equal to	if [\$a != \$b]	if (\$a != \$b)
zero length or null	if [-z \$a]	if (\$%a == 0)
non zero length	if [-n \$a]	if (\$%a > 0)

File Test & Logical Operators

File Test Operators		
Operation	bash	tcsh
file exists	if [-e .bashrc]	if (-e .tcshrc)
file is a regular file	if [-f .bashrc]	
file is a directory	if [-d /home]	if (-d /home)
file is not zero size	if [-s .bashrc]	if (! -z .tcshrc)
file has read permission	if [-r .bashrc]	if (-r .tcshrc)
file has write permission	if [-w .bashrc]	if (-w .tcshrc)
file has execute permission	if [-x .bashrc]	if (-x .tcshrc)

Logical Operators		
Operation	bash	tcsh
Operation	bash	tcsh
NOT	if [! -e .bashrc]	if (! -z .tcshrc)
AND	if [\$a -eq 2] && [\$x -gt \$y]	if (\$a == 2 && \$x <= \$y)
OR	if [[\$a -eq 2 \$x -gt \$y]]	if (\$a == 2 \$x <= \$y)

Examples

- Condition tests using the `if/then` may be nested

```
read a
if [ "$a" -gt 0 ]; then
    if [ "$a" -lt 5 ]; then
        echo "The value of \"$a\" lies somewhere between 0
            and 5"
    fi
fi
```

```
set a = $<
if ( $a > 0 ) then
    if ( $a < 5 ) then
        echo "The value of $a lies somewhere between
            0 and 5"
    endif
endif
```

- This is same as

```
read a
if [[ "$a" -gt 0 && "$a" -lt 5 ]]; then
    echo "The value of $a lies somewhere between 0 and
        5"
fi
OR
if [ "$a" -gt 0 ] && [ "$a" -lt 5 ]; then
    echo "The value of $a lies somewhere between 0 and
        5"
fi
```

```
set a = $<
if ( "$a" > 0 && "$a" < 5 ) then
    echo "The value of $a lies somewhere between 0
        and 5"
endif
```

Loop Constructs

- A *loop* is a block of code that iterates a list of commands as long as the *loop control condition* is true.
- Loop constructs available in

bash: `for`, `while` and `until`

tcsch: `foreach` and `while`

bash: for loops

- The **for** loop is the basic looping construct in **bash**

```
for arg in list
do
    some commands
done
```

- the **for** and **do** lines can be written on the same line: **for** *arg* in *list*; **do**
- **for** loops can also use C style syntax

```
for (( EXP1; EXP2; EXP3 )); do
    some commands
done
```

```
for i in $(seq 1 10)
do
    touch file${i}.dat
done
```

```
for i in $(seq 1 10); do
    touch file${i}.dat
done
```

```
for ((i=1;i<=10;i++))
do
    touch file${i}.dat
done
```


tcsh: foreach loop

- The **foreach** loop is the basic looping construct in **tcsh**

```
foreach arg (list)
    some commands
end
```

```
foreach i ('seq 1 10')
    touch file$i.dat
end
```

while Construct

- The **while** construct tests for a condition at the top of a loop, and keeps looping as long as that condition is true (returns a 0 exit status).
- In contrast to a **for** loop, a **while** loop finds use in situations where the number of loop repetitions is not known beforehand.

bash

```
while [ condition ]
do
    some commands
done
```

tcsh

```
while ( condition )
    some commands
end
```

factorial.sh

```
#!/bin/bash

echo -n "Enter a number less than 10: "
read counter
factorial=1
while [ $counter -gt 0 ]
do
    factorial=$(( $factorial * $counter ))
    counter=$(( $counter - 1 ))
done
echo $factorial
```

factorial.csh

```
#!/bin/tcsh

echo -n "Enter a number less than 10: "
set counter = $<
set factorial = 1
while ( $counter > 0 )
    @ factorial = $factorial * $counter
    @ counter -= 1
end
echo $factorial
```

until Construct (bash only)

- The **until** construct tests for a condition at the top of a loop, and keeps looping as long as that condition is false (opposite of **while** loop).

```
until [ condition is true ]
do
    some commands
done
```

factorial2.sh

```
#!/bin/bash

echo -n "Enter a number less than 10: "
read counter
factorial=1
until [ $counter -le 1 ]; do
    factorial=$(( $factorial * $counter ])
    if [ $counter -eq 2 ]; then
        break
    else
        let counter-=2
    fi
done
echo $factorial
```

Nested Loops

- for, while & until loops can nested. To exit from the loop use the break command

nestedloops.sh

```
#!/bin/bash
## Example of Nested loops

echo "Nested for loops"
for a in $(seq 1 5) ; do
    echo "Value of a in outer loop:" $a
    for b in 'seq 1 2 5' ; do
        c=$((a*b))
        if [ $c -lt 10 ]; then
            echo "a * b = $a * $b = $c"
        else
            echo "$a * $b > 10"
            break
        fi
    done
done
echo "===== "
echo "Nested for and while loops"
for ((a=1;a<=5;a++)); do
    echo "Value of a in outer loop:" $a
    b=1
    while [ $b -le 5 ]; do
        c=$((a*b))
        if [ $c -lt 5 ]; then
            echo "a * b = $a * $b = $c"
        else
            echo "$a * $b > 5"
            break
        fi
        let b+=2
    done
done
echo "===== "
```

nestedloops.csh

```
#!/bin/tcsh
## Example of Nested loops

echo "Nested for loops"
foreach a ('seq 1 5')
    echo "Value of a in outer loop:" $a
    foreach b ('seq 1 2 5')
        @ c = $a * $b
        if ( $c < 10 ) then
            echo "a * b = $a * $b = $c"
        else
            echo "$a * $b > 10"
            break
        endif
    end
end
echo "===== "
echo "Nested for and while loops"
foreach a ('seq 1 5')
    echo "Value of a in outer loop:" $a
    set b = 1
    while ( $b <= 5 )
        @ c = $a * $b
        if ( $c < 5 ) then
            echo "a * b = $a * $b = $c"
        else
            echo "$a * $b > 5"
            break
        endif
        @ b = $b + 2
    end
end
echo "===== "
```

Switching or Branching Constructs I

- The `case` and `select` constructs are technically not loops, since they do not iterate the execution of a code block.
- Like loops, however, they direct program flow according to conditions at the top or bottom of the block.

case construct

```
case variable in
  "condition1")
    some command
  ;;
  "condition2")
    some other command
  ;;
esac
```

select construct

```
select variable [ list ]
do
  command
  break
done
```

Switching or Branching Constructs II

- tcsh has the `switch` construct

switch construct

```
switch (arg list)
  case "variable"
    some command
    breaksw
endsw
```

dooper.sh

```
#!/bin/bash

echo "Print two numbers"
read num1 num2
echo "What operation do you want to do?"

operations='add subtract multiply divide exponentiate
           modulo all quit'
select oper in $operations ; do
  case $oper in
    "add")
      echo "$num1 + $num2 =" ${num1 + $num2}
      ;;
    "subtract")
      echo "$num1 - $num2 =" ${num1 - $num2}
      ;;
    "multiply")
      echo "$num1 * $num2 =" ${num1 * $num2}
      ;;
    "exponentiate")
      echo "$num1 ** $num2 =" ${num1 ** $num2}
      ;;
    "divide")
      echo "$num1 / $num2 =" ${num1 / $num2}
      ;;
    "modulo")
      echo "$num1 % $num2 =" ${num1 % $num2}
      ;;
    "all")
      echo "$num1 + $num2 =" ${num1 + $num2}
      echo "$num1 - $num2 =" ${num1 - $num2}
      echo "$num1 * $num2 =" ${num1 * $num2}
      echo "$num1 ** $num2 =" ${num1 ** $num2}
      echo "$num1 / $num2 =" ${num1 / $num2}
      echo "$num1 % $num2 =" ${num1 % $num2}
      ;;
    *)
      exit
      ;;
  esac
done
```

dooper.csh

```
#!/bin/tcsh

echo "Print two numbers one at a time"
set num1 = <
set num2 = <
echo "What operation do you want to do?"
echo "Enter +, -, x, /, % or all"
set oper = <

switch ( $oper )
  case "x"
    @ prod = $num1 * $num2
    echo "$num1 * $num2 = $prod"
    breaksw
  case "all"
    @ sum = $num1 + $num2
    echo "$num1 + $num2 = $sum"
    @ diff = $num1 - $num2
    echo "$num1 - $num2 = $diff"
    @ prod = $num1 * $num2
    echo "$num1 * $num2 = $prod"
    @ ratio = $num1 / $num2
    echo "$num1 / $num2 = $ratio"
    @ remain = $num1 % $num2
    echo "$num1 % $num2 = $remain"
    breaksw
  case "*"
    @ result = $num1 $oper $num2
    echo "$num1 $oper $num2 = $result"
    breaksw
endsw
```

```
~/Tutorials/BASH/scripts> ./day1/examples/dooper.sh
Print two numbers
1 4
What operation do you want to do?
1) add 3) multiply 5) exponentiate 7) all
2) subtract 4) divide 6) modulo 8) quit
#? 7
1 + 4 = 5
1 - 4 = -3
1 * 4 = 4
1 ** 4 = 1
1 / 4 = 0
1 % 4 = 1
#? 8
```

```
~/Tutorials/BASH/scripts> ./day1/examples/dooper.csh
Print two numbers one at a time
1
5
What operation do you want to do?
Enter +, -, x, /, % or all
all
1 + 5 = 6
1 - 5 = -4
1 * 5 = 5
1 / 5 = 0
1 % 5 = 1
```


dooper1.sh

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

```
echo "Print two numbers"
read num1 num2
echo "What operation do you want to do?"
echo "Options are add, subtract, multiply,
      exponentiate, divide, modulo and all"
read oper

case $oper in
    "add")
        echo "$num1 + $num2 =" ${num1 + $num2}
        ;;
    "subtract")
        echo "$num1 - $num2 =" ${num1 - $num2}
        ;;
    "multiply")
        echo "$num1 * $num2 =" ${num1 * $num2}
        ;;
    "exponentiate")
        echo "$num1 ** $num2 =" ${num1 ** $num2}
        ;;
    "divide")
        echo "$num1 / $num2 =" ${num1 / $num2}
        ;;
    "modulo")
        echo "$num1 % $num2 =" ${num1 % $num2}
        ;;
    "all")
        echo "$num1 + $num2 =" ${num1 + $num2}
        echo "$num1 - $num2 =" ${num1 - $num2}
        echo "$num1 * $num2 =" ${num1 * $num2}
        echo "$num1 ** $num2 =" ${num1 ** $num2}
        echo "$num1 / $num2 =" ${num1 / $num2}
        echo "$num1 % $num2 =" ${num1 % $num2}
        ;;
    *)
        exit
        ;;
esac
```

```
~/Tutorials/BASH/scripts> ./day1/examples/dooper1.sh
Print two numbers
2 5
What operation do you want to do?
Options are add, subtract, multiply, exponentiate,
      divide, modulo and all
all
2 + 5 = 7
2 - 5 = -3
2 * 5 = 10
2 ** 5 = 32
2 / 5 = 0
2 % 5 = 2
```

Arrays I

- **bash** and **tcsch** supports one-dimensional arrays.
- Array elements may be initialized with the `variable[xx]` notation
`variable[xx]=1`
- Initialize an array during declaration

```
bash name=(firstname 'last name')
```

```
tcsch set name = (firstname 'last name')
```

- reference an element `i` of an array `name`
`${name[i]}`
- print the whole array

```
bash ${name[@]}
```

```
tcsch ${name}
```

- print length of array

```
bash ${#name[@]}
```

```
tcsch ${#name}
```

Arrays II

- print length of element `i` of array `name`

```
${#name[i]}
```

Note: In **bash** `${#name}` prints the length of the first element of the array

- Add an element to an existing array

```
bash name=(title ${name[@]})
```

```
tcsh set name = ( title "${name}")
```

- In **tcsh** everything within `"..."` is one variable.
- In the above **tcsh** example, `title` is first element of new array while the second element is the old array `name`
- copy an array `name` to an array `user`

```
bash user=(${name[@]})
```

```
tcsh set user = ( ${name} )
```

Arrays III

- concatenate two arrays

```
bash nameuser=(${name[@]} ${user[@]})
```

```
tcsch set nameuser=( ${name} ${user} )
```

- delete an entire array

```
unset name
```

- remove an element *i* from an array

```
bash unset name[i]
```

```
tcsch  @ j = $i - 1
```

```
        @ k = $i + 1
```

```
        set name = ( ${name[1-$j]} ${name[$k-]} )
```

bash the first array index is zero (0)

tcsch the first array index is one (1)

Arrays IV

name.sh

```
#!/bin/bash

echo "Print your first and last name"
read firstname lastname

name=( $firstname $lastname )

echo "Hello " ${name[@]}

echo "Enter your salutation"
read title

echo "Enter your suffix"
read suffix

name=( $title "${name[@]}" $suffix )
echo "Hello " ${name[@]}

unset name[2]
echo "Hello " ${name[@]}
```

```
~/Tutorials/BASH/scripts/day1/examples> ./name.sh
Print your first and last name
Alex Pacheco
Hello Alex Pacheco
Enter your salutation
Dr.
Enter your suffix
the first
Hello Dr. Alex Pacheco the first
Hello Dr. Alex the first
```

name.csh

```
#!/bin/tcsh

echo "Print your first name"
set firstname = $<
echo "Print your last name"
set lastname = $<

set name = ( $firstname $lastname )
echo "Hello " ${name}

echo "Enter your salutation"
set title = $<

echo "Enter your suffix"
set suffix = "$<"

set name = ( $title $name $suffix )
echo "Hello " ${name}

@ i = $#name
set name = ( $name[1-2] $name[4-$i] )
echo "Hello " ${name}
```

```
~/Tutorials/BASH/scripts/day1/examples> ./name.csh
Print your first name
Alex
Print your last name
Pacheco
Hello Alex Pacheco
Enter your salutation
Dr.
Enter your suffix
the first
Hello Dr. Alex Pacheco the first
Hello Dr. Alex the first
```

Command Line Arguments

- Similar to programming languages, **bash** (and other shell scripting languages) can also take command line arguments
 - `./scriptname arg1 arg2 arg3 arg4 ...`
 - `$0,$1,$2,$3, etc:` positional parameters corresponding to `./scriptname,arg1,arg2,arg3,arg4,...` respectively
 - `$#`: number of command line arguments
 - `$*`: all of the positional parameters, seen as a single word
 - `@`: same as `*` but each parameter is a quoted string.
 - `shift N`: shift positional parameters from `N+1` to `$#` are renamed to variable names from `$1` to `$# - N + 1`
- In **csh**,**tcsh**
 - an array `argv` contains the list of arguments with `argv[0]` set to name of script.
 - `#argv` is the number of arguments i.e. length of `argv` array.

shift.sh

```
#!/bin/bash

USAGE="USAGE: $0 <at least 1 argument>"

if [[ "$#" -lt 1 ]]; then
    echo $USAGE
    exit
fi

echo "Number of Arguments: " $#
echo "List of Arguments: " $@
echo "Name of script that you are running: " $0
echo "Command You Entered:" $0 $*

while [ "$#" -gt 0 ]; do
    echo "Argument List is: " $@
    echo "Number of Arguments: " $#
    shift
done
```

```
dyn100085:examples apacheco$./shift.sh $(seq 1 5)
Number of Arguments: 5
List of Arguments: 1 2 3 4 5
Name of script that you are running: ./shift.sh
Command You Entered: ./shift.sh 1 2 3 4 5
Argument List is: 1 2 3 4 5
Number of Arguments: 5
Argument List is: 2 3 4 5
Number of Arguments: 4
Argument List is: 3 4 5
Number of Arguments: 3
Argument List is: 4 5
Number of Arguments: 2
Argument List is: 5
Number of Arguments: 1
```

shift.csh

```
#!/bin/tcsh

set USAGE="USAGE: $0 <at least 1 argument>"

if ( "$#argv" < 1 ) then
    echo $USAGE
    exit
endif

echo "Number of Arguments: " $#argv
echo "List of Arguments: " ${argv}
echo "Name of script that you are running: " $0
echo "Command You Entered:" $0 ${argv}

while ( "$#argv" > 0 )
    echo "Argument List is: " $*
    echo "Number of Arguments: " $#argv
    shift
end
```

```
dyn100085:examples apacheco$./shift.csh $(seq 1 5)
Number of Arguments: 5
List of Arguments: 1 2 3 4 5
Name of script that you are running: ./shift.csh
Command You Entered: ./shift.csh 1 2 3 4 5
Argument List is: 1 2 3 4 5
Number of Arguments: 5
Argument List is: 2 3 4 5
Number of Arguments: 4
Argument List is: 3 4 5
Number of Arguments: 3
Argument List is: 4 5
Number of Arguments: 2
Argument List is: 5
Number of Arguments: 1
```

Declare command

- Use the **declare** command to set variable and functions attributes.
- Create a constant variable i.e. read only variable

Syntax:

```
declare -r var
```

```
declare -r varName=value
```

- Create an integer variable

Syntax:

```
declare -i var
```

```
declare -i varName=value
```

- You can carry out arithmetic operations on variables declared as integers

```
~/Tutorials/BASH> j=10/5 ; echo $j
10/5
~/Tutorials/BASH> declare -i j; j=10/5 ; echo $j
2
```


Functions I

- Like "real" programming languages, **bash** has functions.
- A function is a subroutine, a code block that implements a set of operations, a "black box" that performs a specified task.
- Wherever there is repetitive code, when a task repeats with only slight variations in procedure, then consider using a function.

```
function function_name {  
    command  
}  
OR  
function_name () {  
    command  
}
```

Functions II

shift10.sh

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

```
usage () {  
    echo "USAGE: $0 [atleast 11 arguments]"  
    exit  
}
```

```
[[ "$#" -lt 11 ]] && usage
```

```
echo "Number of Arguments: " $#  
echo "List of Arguments: " $@  
echo "Name of script that you are running: " $0  
echo "Command You Entered:" $0 $*  
echo "First Argument" $1  
echo "Tenth and Eleventh argument" $10 $11 ${10}  
    ${11}
```

```
echo "Argument List is: " $@  
echo "Number of Arguments: " $#  
shift 9  
echo "Argument List is: " $@  
echo "Number of Arguments: " $#
```

```
dyn100085:examples apacheco$ ./shift10.sh  
USAGE: ./shift10.sh [atleast 11 arguments]  
dyn100085:examples apacheco$ ./shift10.sh $(seq 1 10)  
USAGE: ./shift10.sh [atleast 11 arguments]  
dyn100085:examples apacheco$ ./shift10.sh 'seq 1 2 22'  
Number of Arguments: 11  
List of Arguments: 1 3 5 7 9 11 13 15 17 19 21  
Name of script that you are running: ./shift10.sh  
Command You Entered: ./shift10.sh 1 3 5 7 9 11 13 15 17 19  
21  
First Argument 1  
Tenth and Eleventh argument 10 11 19 21  
Argument List is: 1 3 5 7 9 11 13 15 17 19 21  
Number of Arguments: 11  
Argument List is: 19 21  
Number of Arguments: 2  
dyn100085:examples apacheco$ ./shift10.sh $(seq 21 2 44)  
Number of Arguments: 12  
List of Arguments: 21 23 25 27 29 31 33 35 37 39 41 43  
Name of script that you are running: ./shift10.sh  
Command You Entered: ./shift10.sh 21 23 25 27 29 31 33 35  
37 39 41 43  
First Argument 21  
Tenth and Eleventh argument 210 211 39 41  
Argument List is: 21 23 25 27 29 31 33 35 37 39 41 43  
Number of Arguments: 12  
Argument List is: 39 41 43  
Number of Arguments: 3
```

Functions III

- You can also pass arguments to a function.
- All function parameters or arguments can be accessed via \$1, \$2, \$3,..., \$N.
- \$0 always point to the shell script name.
- \$* or @\$ holds all parameters or arguments passed to the function.
- \$# holds the number of positional parameters passed to the function.
- Array variable called **FUNCNAME** contains the names of all shell functions currently in the execution call stack.
- By default all variables are global.
- Modifying a variable in a function changes it in the whole script.
- You can create a local variables using the **local** command

Syntax:

```
local var=value
```

```
local varName
```

Functions IV

- A function may recursively call itself even without use of local variables.

factorial3.sh

```
#!/bin/bash

usage () {
    echo "USAGE: $0 <integer>"
    exit
}

factorial() {
    local i=$1
    local f

    declare -i i
    declare -i f

    if [[ "$i" -le 2 && "$i" -ne 0 ]]; then
        echo $i
    elif [[ "$i" -eq 0 ]]; then
        echo 1
    else
        f=$(( $i - 1 ))
        f=$( factorial $f )
        f=$(( $f * $i ))
        echo $f
    fi
}

if [[ "$#" -eq 0 ]]; then
    usage
else
    for i in $@ ; do
        x=$( factorial $i )
        echo "Factorial of $i is $x"
    done
fi
```

```
dyn100085:examples apacheco$ ./factorial3.sh $(seq 1 2 11)
Factorial of 1 is 1
Factorial of 3 is 6
Factorial of 5 is 120
Factorial of 7 is 5040
Factorial of 9 is 362880
Factorial of 11 is 39916800
```

Scripting for Job Submission

Problem Description

- I have to run more than one serial job.
 - Solution: Create a script that will submit and run multiple serial jobs.
- I don't want to submit multiple jobs using the serial queue since
 - Cluster Admins give lower priority to jobs that are not parallelized
 - The number of jobs that I want to run exceed the maximum number of jobs that I can run simultaneously
- How do I submit *one* job which can run multiple serial jobs?

One Solution of many

- Write a script which will log into all unique nodes and run your serial jobs in background.
- Easy said than done
- What do you need to know?
 - 1 Shell Scripting
 - 2 How to run a job in background
 - 3 Know what the `wait` command does

```

[alp514.sol](1012): cat checknodes.slr
#!/bin/bash
#
#SBATCH --partition=1ts
#SBATCH --ntasks-per-node=4
#SBATCH --nodes=4
#SBATCH --time=5
#SBATCH --output=nodetest.out
#SBATCH --error=nodetest.err
#SBATCH --job-name=testing
#

export WORK_DIR=${SLURM_SUBMIT_DIR}
srun -s hostname > hostfile
export NPROCS='wc -l hostfile |gawk '://{print $1}''

NODES=('cat hostfile' )
UNODES=('sort hostfile | uniq' )

echo "Nodes Available: " ${NODES[@]}
echo "Unique Nodes Available: " ${UNODES[@]}

echo "Get Hostnames for all processes"
i=0
for nodes in "${NODES[@]"; do
    ssh -n $nodes 'echo $HOSTNAME '$i' ' &
    let i=i+1
done
wait

echo "Get Hostnames for all unique nodes"
i=0
NPROCS='sort hostfile | uniq | wc -l |gawk '://{print $1}''
let NPROCS-=1
while [ $i -le $NPROCS ] ; do
    ssh -n ${UNODES[$i]} 'echo $HOSTNAME '$i' '
    let i=i+1
done

[alp514.sol](1013): sbatch -p imlab checknodes.slr
Submitted batch job 620045

```

```
[alp514.sol](1014): cat nodetest.out
Nodes Available:  sol-b411 sol-b411 sol-b411 sol-b411 sol-b413 sol-b412 sol-b501 sol-b413 sol-b413 sol-b413
                  sol-b412 sol-b412 sol-b412 sol-b501 sol-b501 sol-b501
Unique Nodes Available:  sol-b411 sol-b412 sol-b413 sol-b501
Get Hostnames for all processes
sol-b501 14
sol-b501 6
sol-b501 15
sol-b501 13
sol-b413 4
sol-b413 9
sol-b412 11
sol-b412 10
sol-b413 7
sol-b413 8
sol-b412 5
sol-b411 1
sol-b412 12
sol-b411 3
sol-b411 2
sol-b411 0
Get Hostnames for all unique nodes
sol-b411 0
sol-b412 1
sol-b413 2
sol-b501 3
```

Unix Utilities

- **grep** is a Unix utility that searches through either information piped to it or files in the current directory.
- **egrep** is extended grep, same as **grep -E**
- Use **zgrep** for compressed files.
- **Usage:** **grep <options> <search pattern> <files>**
- Commonly used options

Option	Operation
-i	ignore case during search
-r	search recursively
-v	invert match i.e. match everything except pattern
-l	list files that match pattern
-L	list files that do not match pattern
-n	prefix each line of output with the line number within its input file.
-A num	print num lines of trailing context after matching lines.
-B num	print num lines of leading context before matching lines.

- sed (“stream editor”) is Unix utility for parsing and transforming text files.
- sed is line-oriented, it operates one line at a time and allows regular expression matching and substitution.
- sed has several commands, the most commonly used command and sometime the only one learned is the substitution command, *s*

```
~/Tutorials/BASH/scripts/day1/examples> cat hello.sh | sed 's/bash/tcsh/g'
#!/bin/tcsh
# My First Script
echo 'Hello World!'
```

- List of sed pattern flags and commands line options

Pattern	Operation	Command	Operation
s	substitution	-e	combine multiple commands
g	global replacement	-f	read commands from file
p	print	-h	print help info
I	ignore case	-n	disable print
d	delete	-V	print version info
G	add newline	-i	in file substitution
w	write to file		
x	exchange pattern with hold buffer		
h	copy pattern to hold buffer		

- sed one-liners: <http://sed.sourceforge.net/sed1line.txt>
- sed is a handy utility very useful for writing scripts for file manipulation.

awk programming

- The Awk text-processing language is useful for such tasks as:
 - ★ Tallying information from text files and creating reports from the results.
 - ★ Adding additional functions to text editors like “vi”.
 - ★ Translating files from one format to another.
 - ★ Creating small databases.
 - ★ Performing mathematical operations on files of numeric data.
- Awk has two faces:
 - ★ it is a utility for performing simple text-processing tasks, and
 - ★ it is a programming language for performing complex text-processing tasks.
- awk comes in three variations
 - awk : Original AWK by A. Aho, B. W. Kernighan and P. Weinberger
 - nawk : New AWK, AT&T's version of AWK
 - gawk : GNU AWK, all linux distributions come with gawk. In some distros, awk is a symbolic link to gawk.
- Simplest form of using awk
 - ◆ **awk** *pattern* {*action*}
 - ◆ Most common action: **print**
 - ◆ Print file dosum.sh: **awk** '{print \$0}' dosum.sh
 - ◆ Print line matching bash in all files in current directory:
awk '/bash/{print \$0}' *.sh

- awk patterns may be one of the following

BEGIN : special pattern which is not tested against input.

Mostly used for preprocessing, setting constants, etc. before input is read.

END : special pattern which is not tested against input.

Mostly used for postprocessing after input has been read.

/regular expression/ : the associated regular expression is matched to each input line that is read

relational expression : used with the if, while relational operators

&& : logical AND operator used as pattern1 && pattern2.

Execute action if pattern1 and pattern2 are true

|| : logical OR operator used as pattern1 || pattern2.

Execute action if either pattern1 or pattern2 is true

! : logical NOT operator used as !pattern.

Execute action if pattern is not matched

?: : Used as pattern1 ? pattern2 : pattern3.

If pattern1 is true use pattern2 for testing else use pattern3

pattern1, pattern2 : Range pattern, match all records starting with record that matches

pattern1 continuing until a record has been reached that matches pattern2

- *print expression* is the most common action in the awk statement. If formatted output is required, use the *printf format, expression* action.
- Format specifiers are similar to the C-programming language

%d,%i : decimal number

%e,%E : floating point number of the form [-]d.dddddd.e[±]dd. The %E format uses E instead of e.

%f : floating point number of the form [-]ddd.dddddd

%g,%G : Use %e or %f conversion with nonsignificant zeros truncated. The %G format uses %E instead of %e

%s : character string

- Format specifiers have additional parameter which may lie between the % and the control letter

0 : A leading 0 (zero) acts as a flag, that indicates output should be padded with zeroes instead of spaces.

width : The field should be padded to this width. The field is normally padded with spaces. If the 0 flag has been used, it is padded with zeroes.

.prec : A number that specifies the precision to use when printing.

- string constants supported by awk

**** : Literal backslash

\n : newline

\r : carriage-return

\t : horizontal tab

\v : vertical tab

```
~/Tutorials/BASH/scripts/day1/examples> echo hello 0.2485 5 | awk '{printf "'%s \t %f \n %d \v %0.5d\n'", $1, $2, $3, $3}'
```

```
hello      0.248500
5
      00005
```

- The print command puts an explicit newline character at the end while the printf command does not.

- awk has in-built support for arithmetic operations

Operation	Operator
Addition	+
Subtraction	-
Multiplication	*
Division	/
Exponentiation	**
Modulo	%

Assignment Operation	Operator
Autoincrement	++
Autodecrement	--
Add result to variable	+=
Subtract result from variable	-=
Multiple variable by result	*=
Divide variable by result	/=

```
~/Tutorials/BASH/scripts/day1/examples> echo | awk '{print 10%3}'
1
~/Tutorials/BASH/scripts/day1/examples> echo | awk '{a=10;print a/=5}'
2
```

- awk also supports trigonometric functions such as $\sin(\text{expr})$ and $\cos(\text{expr})$ where expr is in radians and $\text{atan2}(y/x)$ where y/x is in radians

```
~/Tutorials/BASH/scripts/day1/examples> echo | awk '{pi=atan2(1,1)*4;print pi,sin(pi),cos(pi)}'
3.14159 1.22465e-16 -1
```

- Other Arithmetic operations supported are

`exp(expr)` : The exponential function

`int(expr)` : Truncates to an integer

`log(expr)` : The natural Logarithm function

`sqrt(expr)` : The square root function

`rand()` : Returns a random number N between 0 and 1 such that $0 \leq N < 1$

`srand(expr)` : Uses `expr` as a new seed for random number generator. If `expr` is not provided, time of day is used.

- **awk** supports the if and while conditional and for loops
- if and while conditionals work similar to that in C-programming

```
if ( condition ) {  
    command1 ;  
    command2  
}
```

```
while ( condition ) {  
    command1 ;  
    command2  
}
```


- awk supports if ... else if .. else conditionals.

```
if (condition1) {  
    command1 ;  
    command2  
} else if (condition2 ) {  
    command3  
} else {  
    command4  
}
```

- Relational operators supported by if and while

== : Is equal to
!= : Is not equal to
> : Is greater than
>= : Is greater than or equal to
< : Is less than
<= : Is less than or equal to
~ : String Matches to
!~ : Doesn't Match

```
~/Tutorials/BASH/scripts/day1/examples> awk 'if (NR > 0){print NR,":", $0}}' hello.sh  
1 : #!/bin/bash  
2 :  
3 : # My First Script  
4 :  
5 : echo "Hello World!"
```

- The for command can be used for processing the various columns of each line

```
~/Tutorials/BASH/scripts/day1/examples> echo $(seq 1 10) | awk 'BEGIN{a=6}{for (i=1;i<=NF;i++){a+=$i}}END{print a}'  
61
```

- Like all programming languages, awk supports the use of variables. Like Shell, variable types do not have to be defined.
- awk variables can be user defined or could be one of the columns of the file being processed.

```
~/Tutorials/BASH/scripts/day1/examples> awk '{print $1}' hello.sh  
#!/bin/bash  
#  
echo  
~/Tutorials/BASH/scripts/day1/examples> awk '{col=$1;print col,$2}' hello.sh  
#!/bin/bash  
  
# My  
  
echo 'Hello
```

- Unlike Shell, awk variables are referenced as is i.e. no \$ prepended to variable name.
- awk one-liners: <http://www.pement.org/awk/awk1line.txt>

- awk can also be used as a programming language.
- The first line in awk scripts is the shebang line (`#!/`) which indicates the location of the awk binary. Use `which awk` to find the exact location
- On my Linux desktop, the location is `/usr/bin/awk`.
- If unsure, just use `/usr/bin/env awk`

hello.awk

```
#!/usr/bin/awk -f  
  
BEGIN {  
    print "Hello World!"  
}
```

```
~/Tutorials/BASH/scripts/day2/examples> ./hello.awk  
Hello World!
```

- To support scripting, awk has several built-in variables, which can also be used in one line commands
 - `ARGC` : number of command line arguments
 - `ARGV` : array of command line arguments
 - `FILENAME` : name of current input file
 - `FS` : field separator
 - `OFS` : output field separator
 - `ORS` : output record separator, default is newline

- awk permits the use of arrays
- arrays are subscripted with an expression between square brackets ([...])

hello1.awk

```
#!/usr/bin/awk -f

BEGIN {
    x[1] = "Hello,"
    x[2] = "World!"
    x[3] = "\n"
    for (i=1;i<=3;i++)
        printf " %s", x[i]
}
```

```
~/Tutorials/BASH/scripts/day2/examples> ./hello1.awk
Hello, World!
```

- Use the delete command to delete an array element
- awk has in-built functions to aid writing of scripts
 - length** : length() function calculates the length of a string.
 - toupper** : toupper() converts string to uppercase (GNU awk only)
 - tolower** : tolower() converts to lower case (GNU awk only)
 - split** : used to split a string. Takes three arguments: the string, an array and a separator
 - gsub** : add primitive sed like functionality. Usage gsub(/pattern/, "replacement pattern", string)

`getline` : force reading of new line

- Similar to bash, GNU awk also supports user defined function

```
#!/usr/bin/gawk -f
{
    if (NF != 4) {
        error("Expected 4 fields");
    } else {
        print;
    }
}
function error ( message ) {
    if (FILENAME != '-') {
        printf("%s: ", FILENAME) > "/dev/tty";
    }
    printf("line # %d, %s, line: %s\n", NR, message, $0) >>
        "/dev/tty";
}
```

getcpmdvels.sh

```
#!/bin/bash

narg=$(#)
if [ $narg -ne 2 ]; then
    echo "2 arguments needed:[Number of atoms] [Velocity file]\n"
    exit 1
fi

natom=$1
vels=$2

cat TRAJECTORY | \
    awk '{ if ( NR % '$natom' == 0){ \
        printf " %s %s %s\n", $5, $6, $7 \
    }else{ \
        printf " %s %s %s", $5, $6, $7 \
    } \
    }' > $vels
```

getengcons.sh

```
#!/bin/bash

GMSOUT=$1
grep 'TIME      MODE' $GMSOUT | head -1 > energy.dat
awk '/      FS      BOHR/{getline;print }' $GMSOUT >> energy.dat
```

```

#!/bin/bash

narg=$(#)
if [ $narg -ne 6 ]; then
    echo "4 arguments needed: [GAMESS output file] [Number of atoms] [Time Step (fs)] [Coordinates file] [
    Velocity file] [Fourier Transform Vel. File]"
    exit 1
fi

gmsout=$1
natoms=$2
deltat=$3
coords=$4
vels=$5
ftvels=$6
au2ang=0.5291771
sec2fs=1e15
mass=mass.dat

rm -rf $vels $coords $ftvels

##### Atomic Masses (needed for MW Velocities) #####
cat $gmsout | sed -n '/ATOMIC ISOTOPES/,/1 ELECTRON/p' | \
    egrep -i = | \
    sed -e 's//=g' | \
    xargs | awk '{for (i=2;i<=NF;i+=2){printf "%s\n",$i;printf "%s\n",$i;printf "%s\n",$i}}' > $mass
## Use the following with grep###
#grep -i -A1 'ATOMIC ISOTOPES' $gmsout | \
# grep -iv atomic | \
# awk '{for (i=2;i<=NF;i+=2){printf "%s\n",$i;printf "%s\n",$i;printf "%s\n",$i}}' > $mass
## Use the following with grep and sed ###
#grep -i -A1 'ATOMIC ISOTOPES' $gmsout | \
# sed -e '/ATOMIC/d' -e 's/[0-9]=/g' | \
# awk '{for (i=1;i<=NF;i+=1){printf "%s\n",$i;printf "%s\n",$i;printf "%s\n",$i}}' > $mass

##### Coordinates and Velocities #####
awk '/
    CARTESIAN COORDINATES / { \
    icount=3; \
    printf "%d\n\n",'$natoms'
    while (getline>0 && icount<=7){ \
        print $0 ;\
        ++icount \
    } \
}' $gmsout | sed '/---/d' > tmp.$$

#egrep -i -A5 'cartesian coordinates' $gmsout | \

```

```
# sed -e '/CARTESIAN/d' -e '/----/d' > tmp.$$
#
cat tmp.$$ | cut -c -42 | \
awk '{if ( NF == 4){ \
    printf " %4.2f %9.6f %9.6f %9.6f\n", $1, $2*'$au2ang', $3*'$au2ang', $4*'$au2ang' \
} else { \
    print $0 \
} \
}' > $coords
cat tmp.$$ | cut -c 42- | sed '/^ */d' | \
awk '{if ( NR % '$natoms' ==0){ \
    printf " %15.8e %15.8e %15.8e\n", $1*'$sec2fs', $2*'$sec2fs', $3*'$sec2fs' \
} \
else { \
    printf " %15.8e %15.8e %15.8e", $1*'$sec2fs', $2*'$sec2fs', $3*'$sec2fs' \
} \
}' > $vels
rm -rf tmp.$$
```

```
octave -q <<EOF
vels=load("$vels");
atmass=load("$mass");
atmass=diag(atmass);
mwvels=vels*atmass;
ftmwvels=abs(fft(mwvels));
N=rows(ftmwvels);
M=columns(ftmwvels);
deltaw=1/N/$deltat;
fid=fopen("$ftvels","w");
for I=[1:N]
    sumft=0;
    for J=[1:M]
        sumft=sumft+ftmwvels(I,J)^2;
    endfor
    fprintf(fid, " %15.8e %21.14e\n", (I-1)*deltaw, sumft);
endfor
fclose(fid);
EOF
```


getmwvels.awk

```
#!/usr/bin/awk -f
BEGIN{
    if(ARGC < 3){
        printf "3 arguments needed:[Gaussian log file] [Number of atoms] [MW Velocity file]\n";
        exit;
    }
    gaulog = ARGV[1];
    natom = ARGV[2];
    vels = ARGV[3];
    delete ARGV[2];
    delete ARGV[3];
}
/^ *MW Cartesian velocity:/ {
    icount=1;
    while((getline > 0)&&icount<=natom+1){
        if(icount>=2){
            gsub(/D/, "E") ;
            printf "%16.8e%16.8e%16.8e", $4, $6, $8 > vels;
        }
        ++icount;
    }
    printf "\n" > vels;
}
```

gettrajxyz.awk

```
#!/usr/bin/awk -f
BEGIN{
    if(ARGC < 3){
        printf "3 arguments needed:[Gaussian log file] [Number of atoms] [Coordinates file]\n";
        exit;
    }
    gauilog = ARGV[1];
    natom = ARGV[2];
    coords = ARGV[3];
    delete ARGV[2];
    delete ARGV[3];
}
/^ *Input orientation:/ {
    icount=1;
    printf "%d\n\n",natom > coords;
    while((getline > 0)&&icount<=natom+4){
        if(icount>=5){
            printf "%5d%16.8f%16.8f%16.8f\n", $2,$4,$5,$6 > coords;
        }
        ++icount;
    }
}
```

Wrap Up

References & Further Reading

- BASH Programming <http://tldp.org/HOWTO/Bash-Prog-Intro-HOWTO.html>
- Advanced Bash-Scripting Guide <http://tldp.org/LDP/abs/html/>
- Regular Expressions <http://www.grymoire.com/Unix/Regular.html>
- AWK Programming <http://www.grymoire.com/Unix/Awk.html>
- awk one-liners: <http://www.pement.org/awk/awk1line.txt>
- sed <http://www.grymoire.com/Unix/Sed.html>
- sed one-liners: <http://sed.sourceforge.net/sed1line.txt>
- CSH Programming <http://www.grymoire.com/Unix/Csh.html>
- csh Programming Considered Harmful
<http://www.faqs.org/faqs/unix-faq/shell/csh-whynot/>
- Wiki Books <http://en.wikibooks.org/wiki/Subject:Computing>