Basic Shell Scripting

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Outlines

- **HPC User Environment 1**

  1. Intro to HPC
  2. Getting started
  3. Into the cluster
  4. Software environment (modules)

- **HPC User Environment 2**

  1. Basic concepts
  2. Preparing my job
  3. Submitting my job
  4. Managing my jobs

Outlines

1. **Introduction**
    1) What's Shell?
    2) What can Shell do?
2. **Basic Knowledge**
    1) Interactive vs Non-interactive (Shell Script)
    2) Basic Commands & Syntax
    3) Variables
    4) Arrays
    5) Arithmetic Operations
3. **Beyond Basics**
    1) Subshells
    2) Flow Control
    3) Advanced Text Processing Commands
4. **BONUS: Where to Get Help**

Outlines

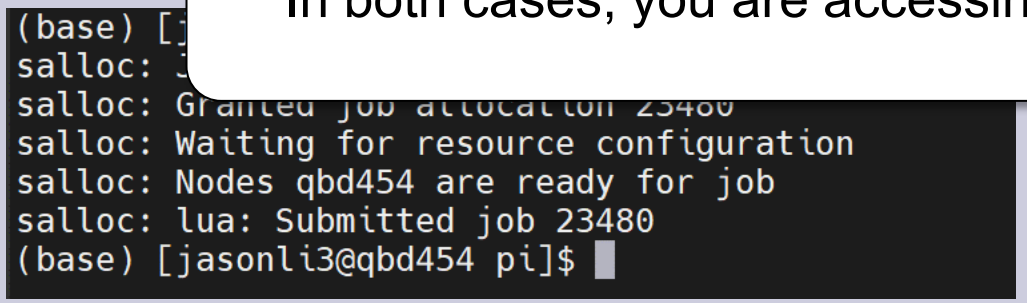
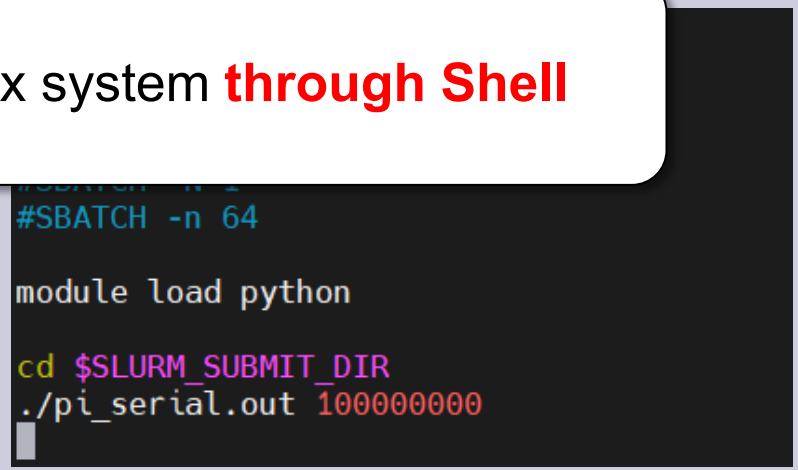
- **Example and exercises:**
  - http://www.hpc.lsu.edu/training/weekly-materials/Downloads/ShellScripting.zip

Outlines

1. **Introduction**
   1) What's Shell?
   2) What can Shell do?
2. **Basic Knowledge**
   1) Interactive vs Non-interactive (Shell Script)
   2) Basic Commands & Syntax
   3) Variables
   4) Arrays
   5) Arithmetic Operations
3. **Beyond Basics**
   1) Subshells
   2) Flow Control
   3) Advanced Text Processing Commands
4. **BONUS: Where to Get Help**

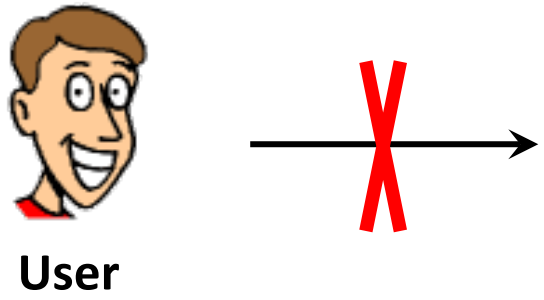
1) What's Shell?

- **Previously in HPC User Environment 2…**
  - Two types of jobs

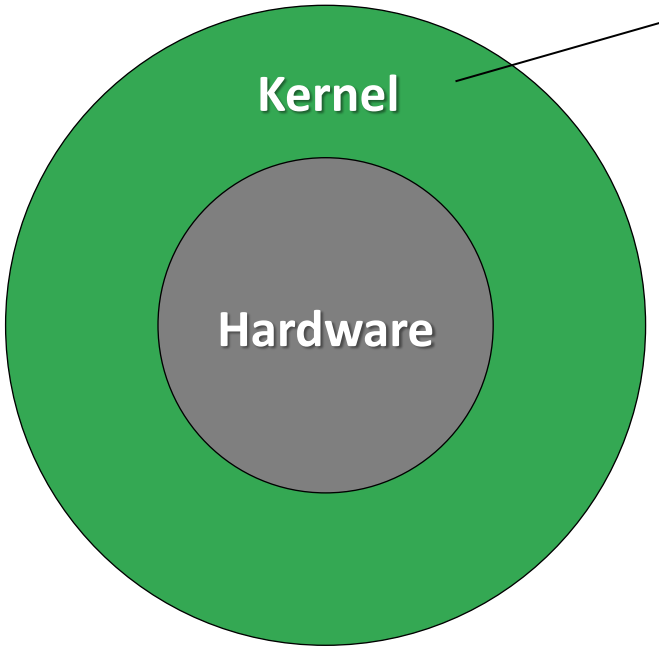
1) Interactive job	2) Batch job
	

In both cases, you are accessing a Linux system **through Shell**

1) What's Shell?



User

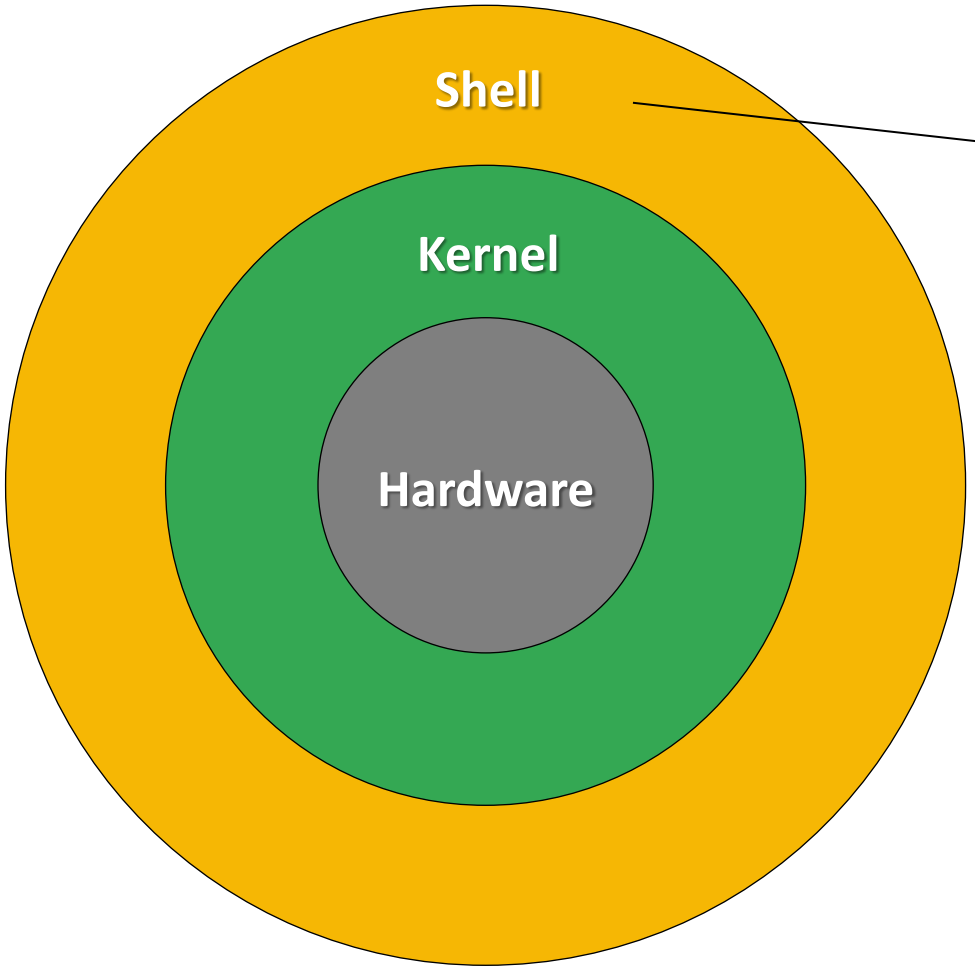


- Resource management
- Process management
- Device Drivers
- System Calls
- …

→ **Speaks: Machine**

1) What's Shell?

User

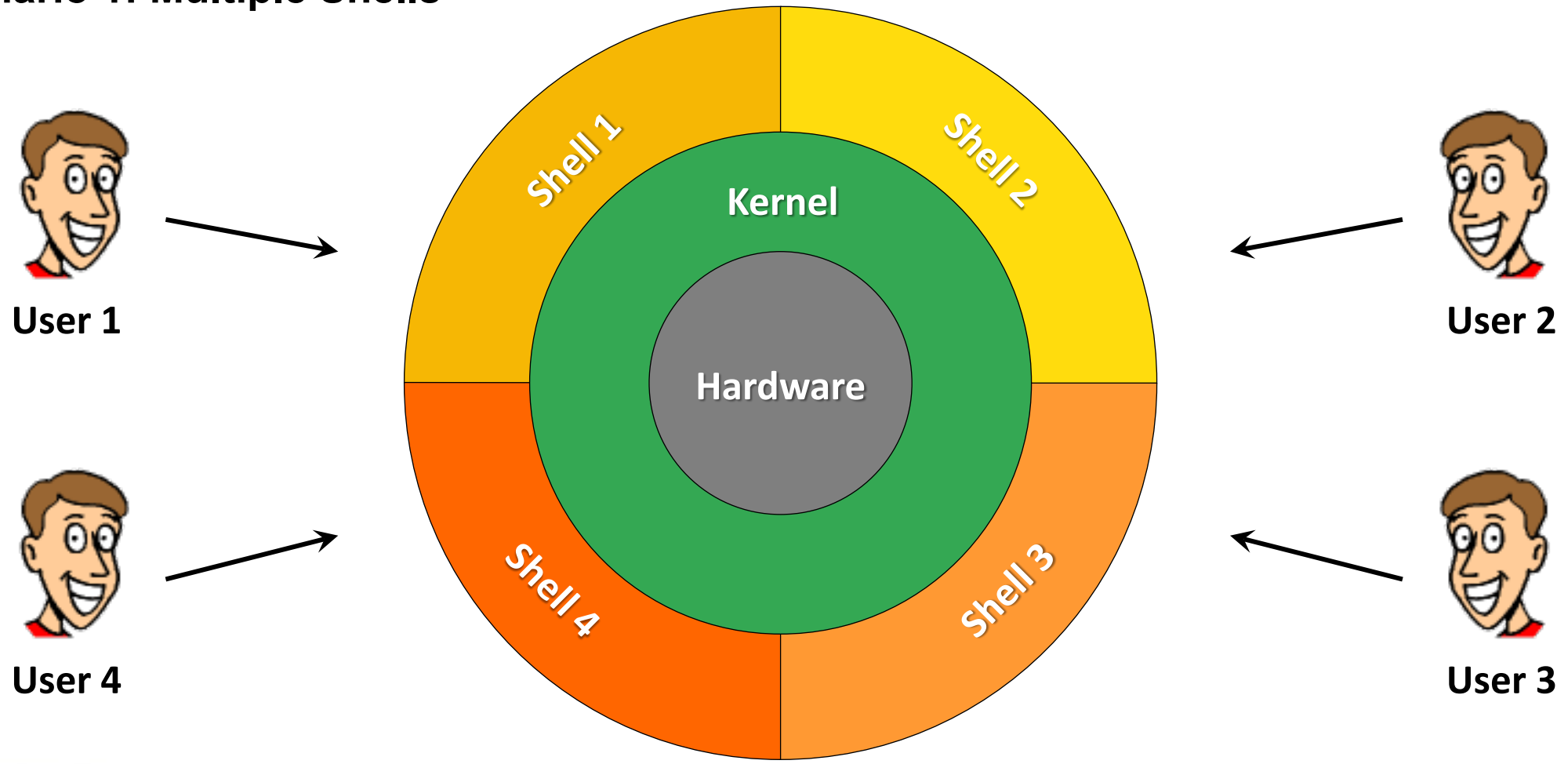


- Command execution
- Scripting
- …

→ **Speaks: Human**

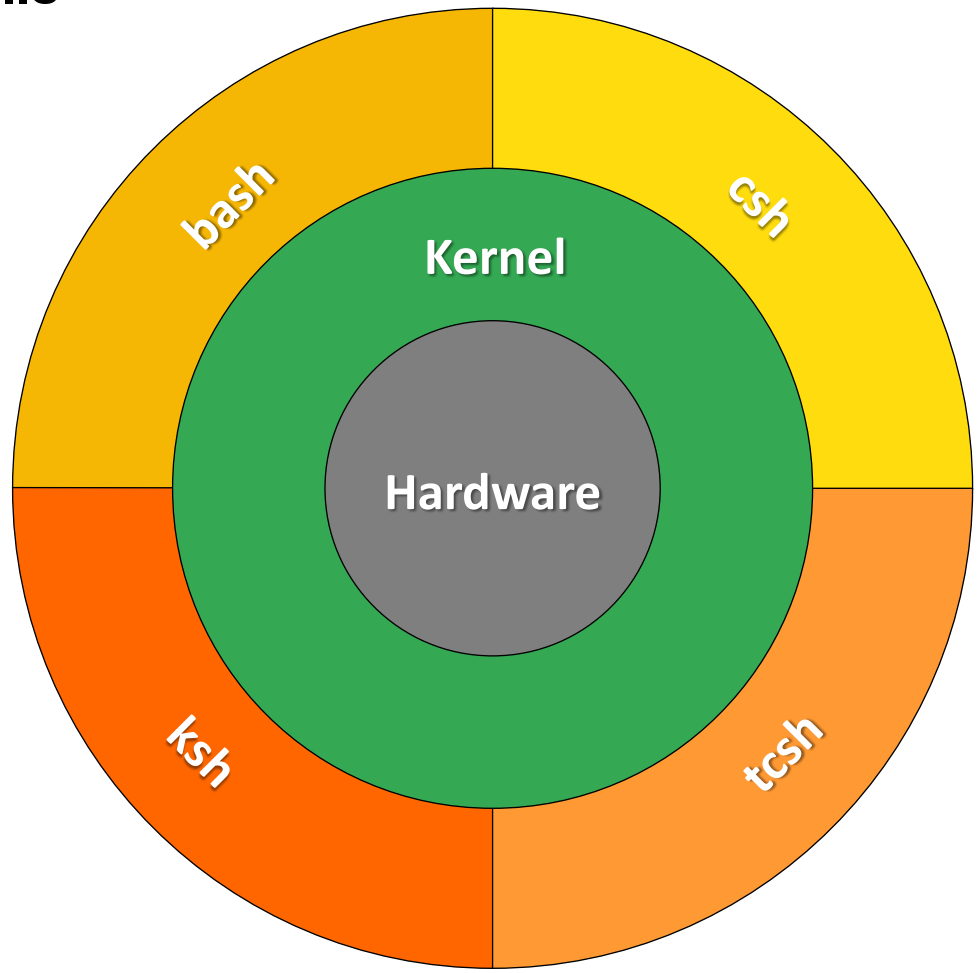
1) What's Shell?

- **Scenario 1: Multiple Shells**



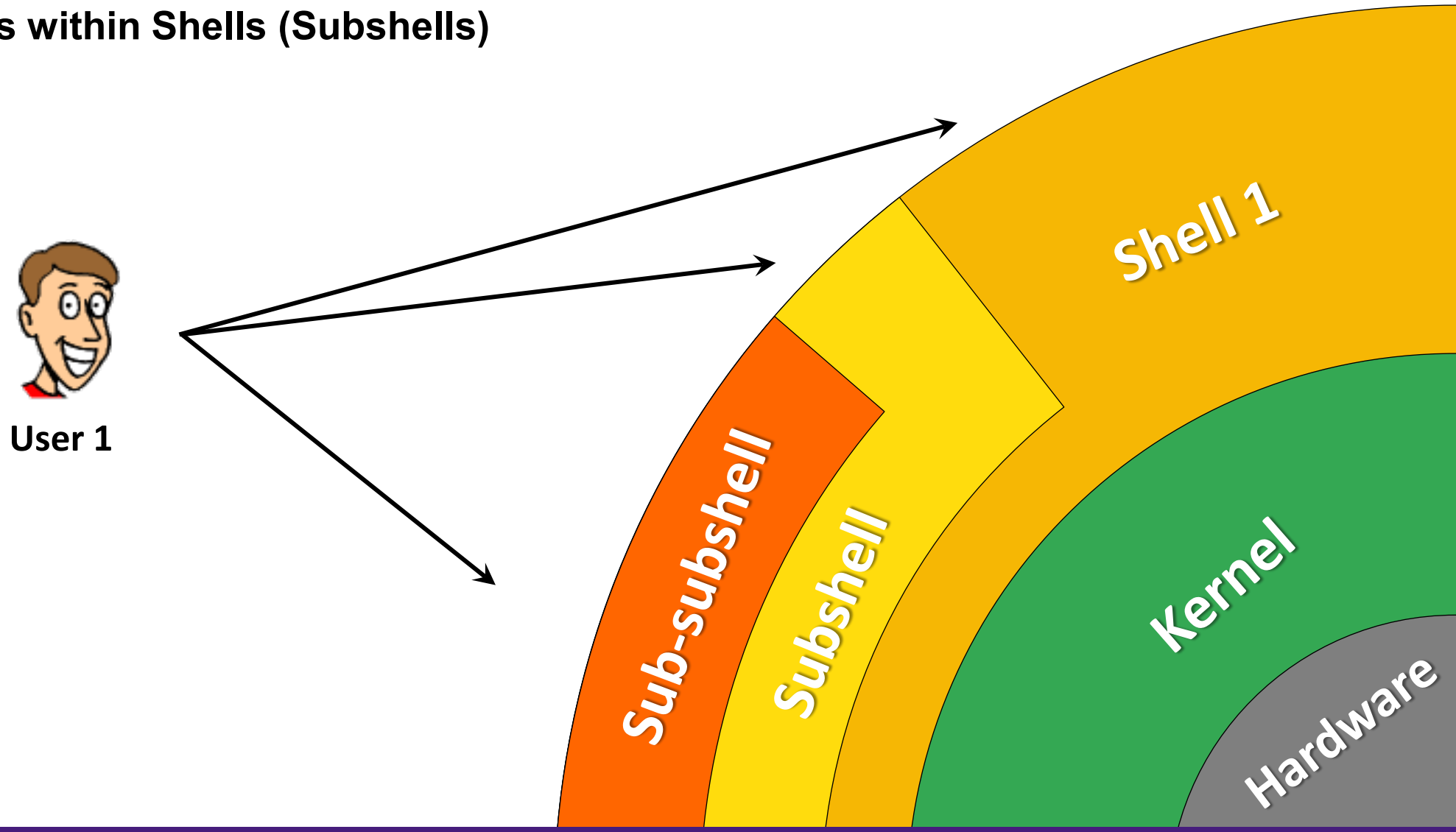
1) What's Shell?

- **Scenario 1: Multiple Shells**



1) What's Shell?

- **Scenario 2: Shells within Shells (Subshells)**



1) What's Shell?

- **Shell:**
  - A **user interface** to access UNIX-like systems (e.g., Linux) by executing commands.

Outlines

2) What can Shell do?

- **Shell can do this …**
  - Typing commands one by one

```
(base) [jasonli3@qbd1 ShellScripting]$ ls
1.1-ShellExamples  1.2-Goal  exec  README.txt
(base) [jasonli3@qbd1 ShellScripting]$ date
Tue Sep 17 15:17:47 CDT 2024
(base) [jasonli3@qbd1 ShellScripting]$ echo $SHELL
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(base) [jasonli3@qbd1 exec]$ ls
pi_bash.sh  pi_c  pi_c.sbatch
(base) [jasonli3@qbd1 exec]$ ./pi_c 100000000
niter=100000000
count in circle:78547994
Pi: 3.141920
(base) [jasonli3@qbd1 exec]$
```

2) What can Shell do?

- **Shell can also do this …**
  - A much more complicated program / script

```
#!/bin/bash

# URL and file name
URL=$1
FILENAME=`basename $URL`

# Number of parts
PARTS=$SLURM_NTASKS
echo "Downloading in $PARTS parts..."

# Create temporary directory for parts
TEMP_DIR=$(mktemp -d)

# Calculate the range for each part
FILE_SIZE=$(curl -sIk $URL | awk '/Content-Length/ {print $2}' | tr -d '\r')  # Get file size
PART_SIZE=$((FILE_SIZE / PARTS))  # Calculate part size
LAST_PART_SIZE=$((FILE_SIZE - PART_SIZE * (PARTS - 1)))  # Calculate size of the last part

# Download each part concurrently
for ((i = 0; i < PARTS; i++)); do
  start=$((i * PART_SIZE))
  end=$((start + PART_SIZE - 1))

  if [[ $i -eq $((PARTS - 1)) ]]; then
    end=$((start + LAST_PART_SIZE - 1))
  fi

  curl -ks -o "$TEMP_DIR/part$i" --range "$start-$end" "$URL" &
done

# Wait for all downloads to finish
wait

# Merge the parts into a single file
for ((i = 0; i < PARTS; i++)); do
  cat "$TEMP_DIR/part$i" >> "data/$FILENAME"
done

# Clean up temporary directory
rm -rf "$TEMP_DIR"

echo "Download completed!"
```

[1] *ShellScripting/1.2-WhatCanShellDo/parallelDownload.sh*

2) What can Shell do?

- **Shell Scripting:**
  - A practice to **automate tasks** with Shell commands.

2) What can Shell do?

- **Take a closer look at this:**

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[1] *ShellScripting/1.2-WhatCanShellDo/parallelDownload.sh*

2) What can Shell do?

- **Take a closer look at this:**

Isn't it basically a programming language?

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[1] *ShellScripting/1.2-WhatCanShellDo/parallelDownload.sh*

2) What can Shell do?

- **Questions:**

a) Why learn **Shell** if I am already familiar with **another language** (Python / C++ / Fortran) ?

b) Why learn **another language** (Python / C++ / Fortran) if I can just use **Shell**?

2) What can Shell do?

a) Why learn Shell if I am already familiar with another language?

– Shell is a "**quick and dirty**" way to get things done!

• *Example*: Change all text "`/ddnB/work`" to "`/work`" in all files in folder "`~/mycode/`" and subfolders.

Python

```python
import os

folder = os.path.expanduser('~/mycode')

for dirpath, _, filenames in os.walk(folder):
    for filename in filenames:
        filepath = os.path.join(dirpath, filename)
        with open(filepath, 'r') as file:
            content = file.read()
        new_content = content.replace('/ddnB/work', '/work')
        with open(filepath, 'w') as file:
            file.write(new_content)
```

Shell

```
find ~/mycode/ -type f -exec sed -i 's|/ddnB/work|/work|g' {} +
```

[1] *ShellScripting/1.2-WhatCanShellDo/pathSwap.py*
[2] *ShellScripting/1.2-WhatCanShellDo/pathSwap.sh*

b) Why learn another language if I can just use Shell?

– Shell is **highly inefficient** for heavy calculation!

• *Example*: Try the pi calculation codes in folder "`ShellScripting/1.2-WhatCanShellDo/`":

C	Shell
`$ ./pi_c 10000`	`$ ./pi_shell.sh 10000`

`(base) [jasonli3@qbd177 1.2-Goal]$ time ./pi_c 10000`
`niter=10000`
`count in circle:7888`
`Pi: 3.155200`
 	
`real 0m0.002s`
`user 0m0.000s`
`sys 0m0.001s`
	`(base) [jasonli3@qbd177 1.2-Goal]$ time ./pi_shell.sh 10000`
	`niter=10000`
	`count in circle:7876`
	`Pi: 3.150400000000000000`
	
	`real 1m7.943s`
	`user 0m27.922s`
	`sys 0m45.868s`

[1] *ShellScripting/1.2-WhatCanShellDo/pi_c*
[2] *ShellScripting/1.2-WhatCanShellDo/pi_shell.sh*

2) What can Shell do?

- **Goal of Shell scripting:**

Shell scripting is NOT for…	Shell scripting IS for…
• **Heavy calculation** (basically, anything you wish to run faster!) • Replacing your known language / software	• **Automating job workflow** with minimum scripting (e.g., set up environment, call proper executables, etc.) • **Pre-processing** / **Post-processing** (e.g., trim data, edit config files in batch, etc.)

- **Goal of this training:**

We do NOT expect you to be…	We DO expect you to be…
• An expert in Linux or Shell language.	• Familiar with Shell's **basic usage**. • Able to use Shell scripting to **optimize job workflow**.

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   4) Arrays
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   2) Flow Control
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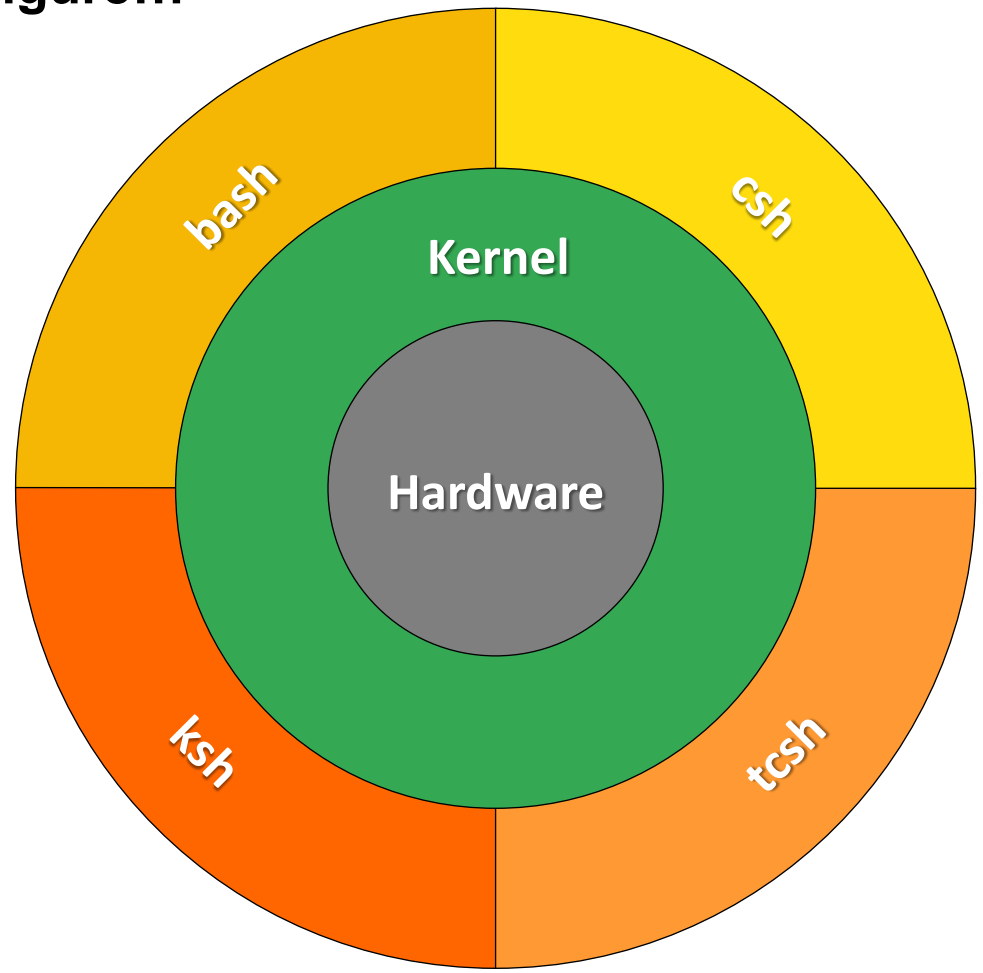
4. BONUS: Where to Get Help

Before we continue…

- **Remember we had this figure…**



Before we continue…

- **There are many Shell implementations**

  - **sh** (Original Bourne Shell)
  - **bash** (Bourne Again Shell)
  - **csh** (C Shell)
  - **tcsh** (TENEX C Shell, more features)
  - **ksh** (KornShell)
  - **zsh** (Z Shell)
  - **dash** (Debian Almquist Shell)
  - **fish** (Friendly Interactive Shell)
  - …

- Supported by our clusters
- Feel free to use whichever you like!
- Can set your own default Shell

Before we continue…

- **There are many Shell implementations**
  - **sh** (Original Bourne Shell)
  - **bash** (Bourne Again Shell)
  - **csh** (C Shell)
  - **tcsh** (TENEX C Shell, more features)
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  - **zsh** (Z Shell)
  - **dash** (Debian Almquist Shell)
  - **fish** (Friendly Interactive Shell)
  - …

- Default Shell on all clusters
- Will only talk about it today

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1) Interactive vs Non-interactive Shell

a) Two ways to access Shell

Interactive

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(base) [jasonli3@qbd1 exec]$ ./pi_c 100000000
niter=100000000
count in circle:78547994
Pi: 3.141920
(base) [jasonli3@qbd1 exec]$
```

Non-interactive

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```

1) Interactive vs Non-interactive Shell

a) Two ways to access Shell

Interactive

- Runs in terminal
- Can interact in real time
- Type commands one-by-one
- E.g., every time you log in in terminal

Non-interactive

```
#!/bin/bash

# URL and file name
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1) Interactive vs Non-interactive Shell

a) Two ways to access Shell

Interactive

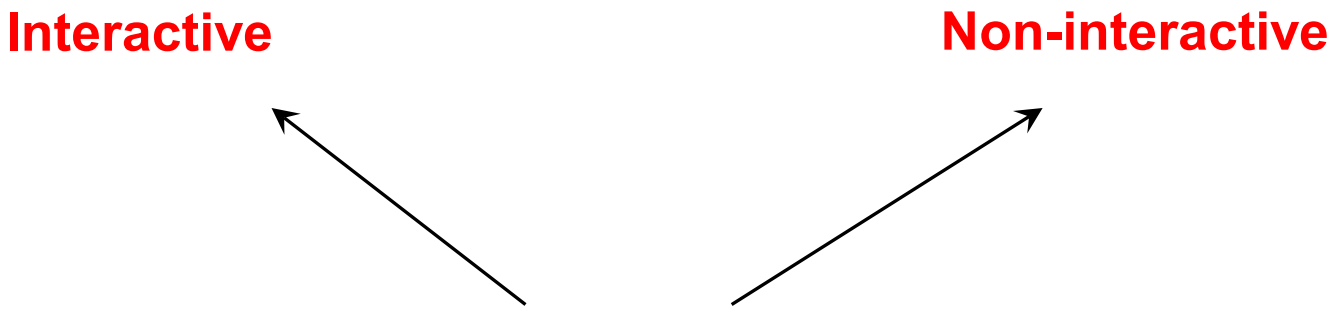
- Runs in terminal
- Can interact in real time
- Type commands one-by-one
- E.g., every time you log in in terminal

Non-interactive

- Prewritten script (Shell script)
- Cannot interact while it is running
- Runs by itself (line-by-line)

1) Interactive vs Non-interactive Shell

a) Two ways to access Shell

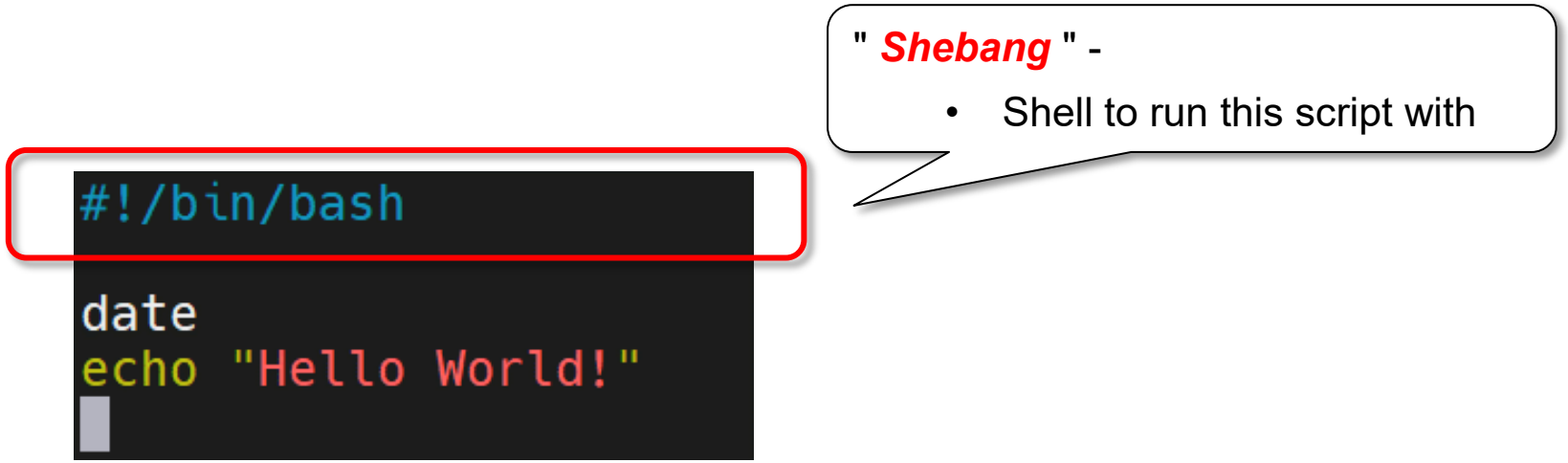


Shell scripting works the same way in both! *

* A few features may be slightly different. But for now, don't worry about that.

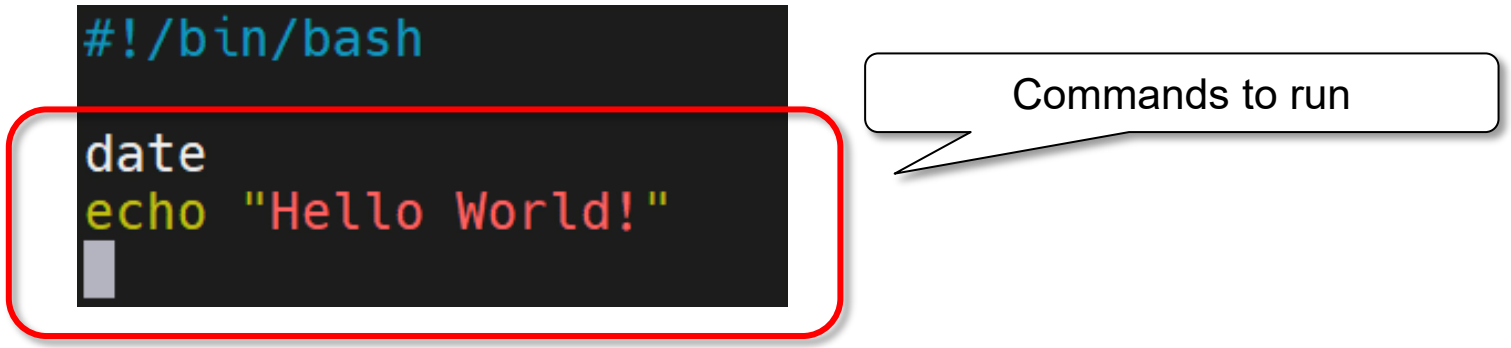
1) Interactive vs Non-interactive Shell

b) How to write a Shell script



[1] *ShellScripting/2.1-InteractiveVsNonInteractive/helloworld.sh*

b) How to write a Shell script



[1] *ShellScripting/2.1-InteractiveVsNonInteractive/helloworld.sh*

1) Interactive vs Non-interactive Shell

c) How to run a Shell script (four methods)

	Method	Example	Remarks
1	**Use full path** (Most common)	`$ ./helloworld.sh` `$ /path/to/helloworld.sh`	• File must be **executable** (Run "`chmod u+x [filename]`" if not) • Uses Shell in **shebang** (if exists) or **default Shell** • Starts a new **subshell**
2	**Use specific Shell**	`$ bash helloworld.sh` `$ csh helloworld.sh`	• File does **NOT** need to be executable • Uses the **specified Shell** (ignore shebang) • Starts a new **subshell**
3	**Use "source" or "."**	`$ source helloworld.sh` `$ . helloworld.sh`	• File does **NOT** need to be executable • Uses **current Shell** (ignore shebang) • Does **NOT** start a new subshell
4	**Run as Shell command**	`$ helloworld.sh`	• File must be **executable** • Uses Shell in **shebang** (if exists) or **default Shell** • Parent directory must be added to **$PATH** environment variable • Starts a new **subshell**

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[1] *ShellScripting/2.1-InteractiveVsNonInteractive/helloworld.sh*

1) Interactive vs Non-interactive Shell

- **Pop quiz: What is this?**

➔ **Anything you learned about Shell today, applies to your batch job files!**

```
#!/bin/bash
#SBATCH -A loni_loniadmin1
#SBATCH -p single
#SBATCH -t 1:00:00
#SBATCH -N 1
#SBATCH -n 12

# Time stamp at the beginning
date

# Run the code
./pi_c 1000000

# Time stamp at the end
date
```

[1] *ShellScripting/2.1-InteractiveVsNonInteractive/pi_c.sbatch*

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a) Basic commands

Command		Description
File	`ls`	List files at a given location .
	`cp` / `mv`	Copy / Move files.
	`rm`	Remove files.
	`find`	Search for files.
Directory	`cd`	Change directory.
	`mkdir`	Create a directory.
	`pwd`	Print current directory in standard output.
Display	`cat`	Print out an entire file in standard output.
	`head` / `tail`	Show first / last several lines of a file.
	`more` / `less`	Display file one page at a time.
System	`echo`	Print out strings in standard output.
	`date`	Print out current date & time in standard output.
...		

[1] https://www.hpc.lsu.edu/training/archive/tutorials.php

2) Basic Commands & Syntax

b) Commonly used special characters that works with commands

Character	Description	Example
#	**Comment**: Anything follows in the same line will not be executed.	`$ date # Print time stamp`
;	**Command separator**: Allows multiple commands in one line.	`$ module purge; module load python`
|	**Pipeline**: Use output of first command as input of the second.	`$ squeue -u $USER | wc -l`
>	**Redirect (Output)**: Redirect standard output / error to file. This method overwrites the file.	`$ ./testoutput > out.txt` `$ ./testoutput 1> out.txt 2> err.txt`
>>	**Redirect (Output)**: Redirect standard output / error to file. This method appends to the file.	`$ ./testoutput >> out.txt` `$ ./testoutput 1>> out.txt 2>> err.txt`
<	**Redirect (Input)**: Read input from a file instead of standard input.	`$ ./testinput < input.txt`
&	**Send to background**: Send a command to background, and do not wait for it to finish.	`$ ./testoutput &`

[1] *ShellScripting/2.2-BasicCommands/testoutput*
[2] *ShellScripting/2.2-BasicCommands/testinput*

Outlines

1. Introduction
   1) What's Shell?
   2) What can Shell do?
2. **Basic Knowledge**
   1) Interactive vs Non-interactive (Shell Script)
   2) Basic Commands & Syntax
   3) Variables
   4) Arrays
   5) Arithmetic Operations
3. Beyond Basics
   1) Subshells
   2) Flow Control
   3) Advanced Text Processing Commands
4. BONUS: Where to Get Help

3) Variables

a) Variable basics

	To assign	To access	To delete
Syntax	`var=value`	`$var`	`unset var`
Examples	`$ str="Hello World!"`	`$ echo $str`	
	`$ workdir="/work/jasonli3/test"`	`$ cd $workdir`	
	`$ myexec="/home/jasonli3/myexec"` `$ myout="/work/jasonli3/out.txt"`	`$ $myexec > $myout`	

– **ATTENTION!**

- All Shell variables are treated as **strings**! (No integer, float, Boolean...)
- **No space** allowed in assignment!
- Use `{ }` to explicitly mark variable name. (e.g., `${var}` instead of `$var`)
  – Think about it. When can this be useful?

b) Naming rules

- Allowed characters: **letters** (`a-z`, `A-Z`), **numbers** (`0-9`), **underscore** (`_`)
- Must begin with a **letter** or an **underscore**.
- No other special characters (e.g., `#`, `@`, `%`, `$`, …)
  - **Allowed**: `varname`, `var_name`, `_varName`, `var123`
  - **Not allowed**: `123var`, `#var`, `var@name`, `var-123`
- Case sensitive
  - `VAR` and `var` are different variables!

c) Global & local variables

	Local	Global
Syntax	`$ var=value`	`$ export VAR=value`
Differences	• Exist only in **current shell**	• **Copied** to all **subshells**
	• Lowercase*	• Uppercase*

* **Convention**, to avoid conflict

d) Environment variables

– **Definition**:

- Specific variables used by Shell or other programs to regulate certain functionalities.

– **Remarks**:

- Names are **specific** (Cannot be other names)
- Usually **global** (Convention)
- **Customizable**, will change Shell or program behavior (Caution!)
- Programs may have their own environment variables (e.g., Conda / Python / R / MPI …)

d) Environment variables

Variable		Functionality
Shell	`USER`	Username.
	`PWD`	Full path to current directory.
	`HOME`	Full path to user's home directory.
	`HOSTNAME`	Name of the current node.
	`PATH`	A list of paths to look for executables as Shell commands (separated by ":").
	`LD_LIBRARY_PATH`	A list of paths to look for shared libraries (separated by ":").
Slurm	`SLURM_JOB_ID`	Slurm job ID.
	`SLURM_JOB_NODELIST`	A list of nodes required for current job (useful for MPI).
OpenMP	`OMP_NUM_THREADS`	Number of threads per process for OpenMP.
…		

[1] https://www.hpc.lsu.edu/docs/slurm.php

e) Quotations & variables

Quotation	Description	Example
""	Allows **variable expansion** ("$") and **command substitution** ("``") within quotes, and preserves literal values of **all other characters**.	`$ echo "echo $USER"` `echo jasonli3`
''	Preserves the literal value of **ALL CHARACTERS** within the quotes.	`$ echo 'echo $USER'` `echo $USER`
``	**Command substitute**: Execute the command(s) inside the quotation and use its output to replace the quotation.	`$ echo `echo $USER`` `jasonli3`

Outlines

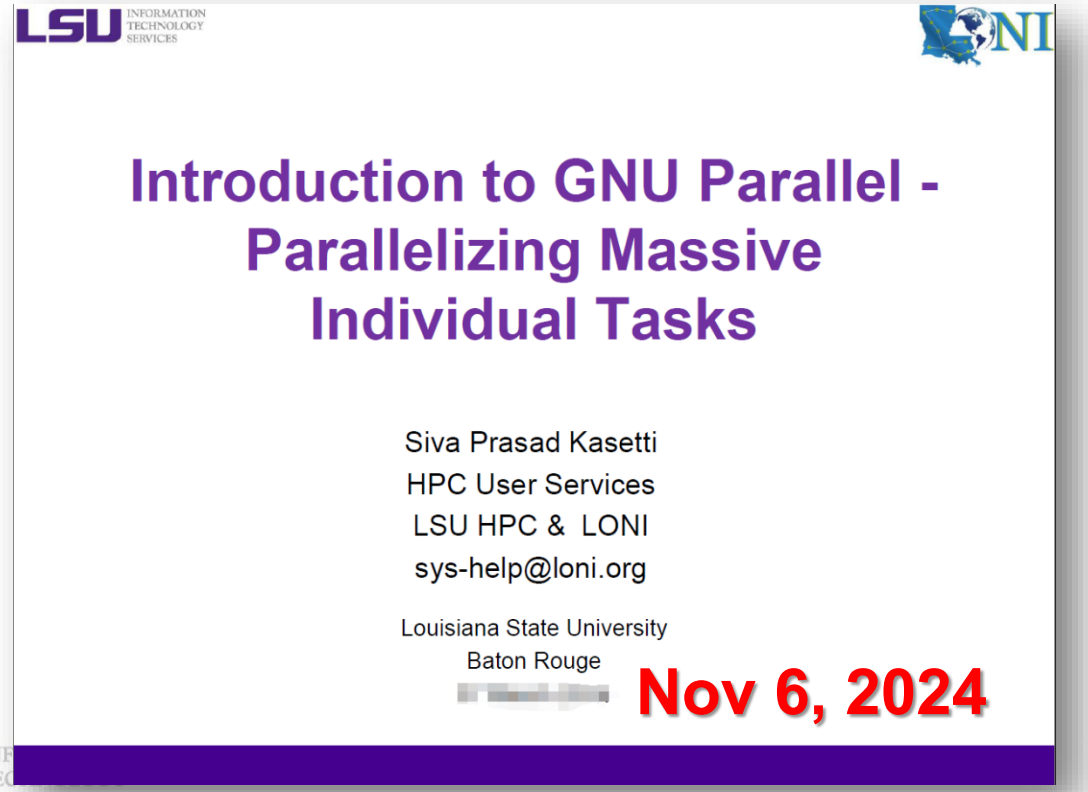
4) Arrays

- **A collection of multiple values**
  - Basic logic very similar to “arrays” in any other language, **with some twists**!
    - Each element is accessed by **index**
    - Index starts with **0**

	To assign	To delete	To access
Entire array	`$ myAry=("Alice" "Bob" "Charlie")`	`$ unset myAry`	`$ echo ${myAry[@]}`
One element	`$ myAry[1]="Brian"`	`$ unset myAry[1]`	`$ echo ${myAry[1]}`

- **Bonus**: Get length of array - `${#myAry[@]}`

- **Question:**
  - I am not using Shell for heavy calculation anyways! What can I possibly need arrays for?



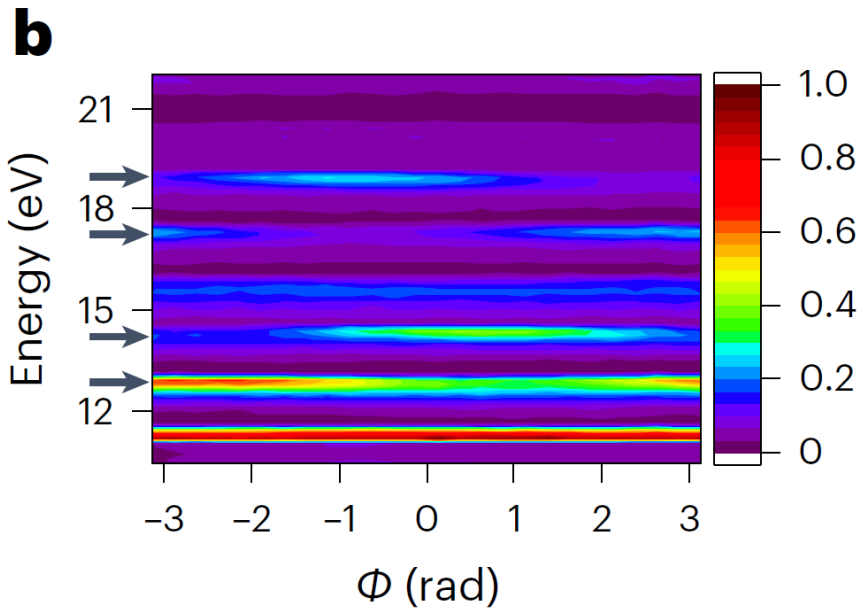

```
$ parallel myexec ::: ${inputParams[@]}
```

[1] https://www.hpc.lsu.edu/training/tutorials.php#upcoming

Outlines

5) Arithmetic Operations

- **Wait a minute!**
  - Didn't you say Shell does **not** support number type, and we should **not** use it for heavy calculation?
  - Correct!
  - But! Sometimes arithmetic is still needed.
    - **Example**: Parallelizing a photoelectron spectrum calculation (my actual research)!
      - Each parallel process labeled w/ an integer index [-100, 100]
      - But! Need to pass on a delay parameter to each process, a float number calculated from the integer index



[1] *Nat. Photon.* **17**, 200–207 (2023). https://doi.org/10.1038/s41566-022-01127-3

5) Arithmetic Operations

- **What does NOT work:**

```
$ a=10
$ b=$a/3+2
$ echo $b      # Guess what you get?
10/3+2
```

[1] *ShellScripting/2.5-Arithmetic/bcExample.txt*

5) Arithmetic Operations

- **What DOES work** (assuming `a=10`):

	Method	Example	Remarks
1	`$((…))` (Most common)	`$ echo $(($a/3+2))`	• Evaluate **everything inside** the braces. • **Integers** only!

2	`let` (Slightly more advanced)	`$ let b=$a/3+2`
		`$ let b=a/3+2`
		`$ let b++`
			• Evaluate **assignment** w/ arithmetic calculation.
			• "`$`" can be emitted.
			• **Integers** only!

3	`expr` (Legacy, most limited)	`$ expr $a / 3 + 2`	• Strictly limited to "`ARG1 OPERATION ARG2`" format. • **Integers** only!

4	`bc` (Most powerful)	`$ bc`
		`scale=3`
		`a=10;a/3+2`
		`$ bc < bcExample.txt`
		`$ echo "$a/2+3" | bc`
			• **Interactive** and **non-interactive** mode.
			• Does **NOT** support Shell syntax (namely, "`$`" for variables).
			• Unassigned variables treated as `0`.
			• `scale` variable determines number of decimals.
			• Supports **float number**!

[1] *ShellScripting/2.5-Arithmetic/bcExample.txt*

Summary

- **In this section, we talked about:**

1) Interactive vs Non-interactive (Shell Script)
2) Basic Commands & Syntax
3) Variables
4) Arrays
5) Arithmetic Operations

Break

- Get some water
- Use restroom
- Ask questions

- Don’t forget, the examples are at:
  - http://www.hpc.lsu.edu/training/weekly-materials/Downloads/ShellScripting.zip

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3. **Beyond Basics**
   1) Subshells
   2) Flow Control
   3) Advanced Text Processing Commands
4. BONUS: Where to Get Help

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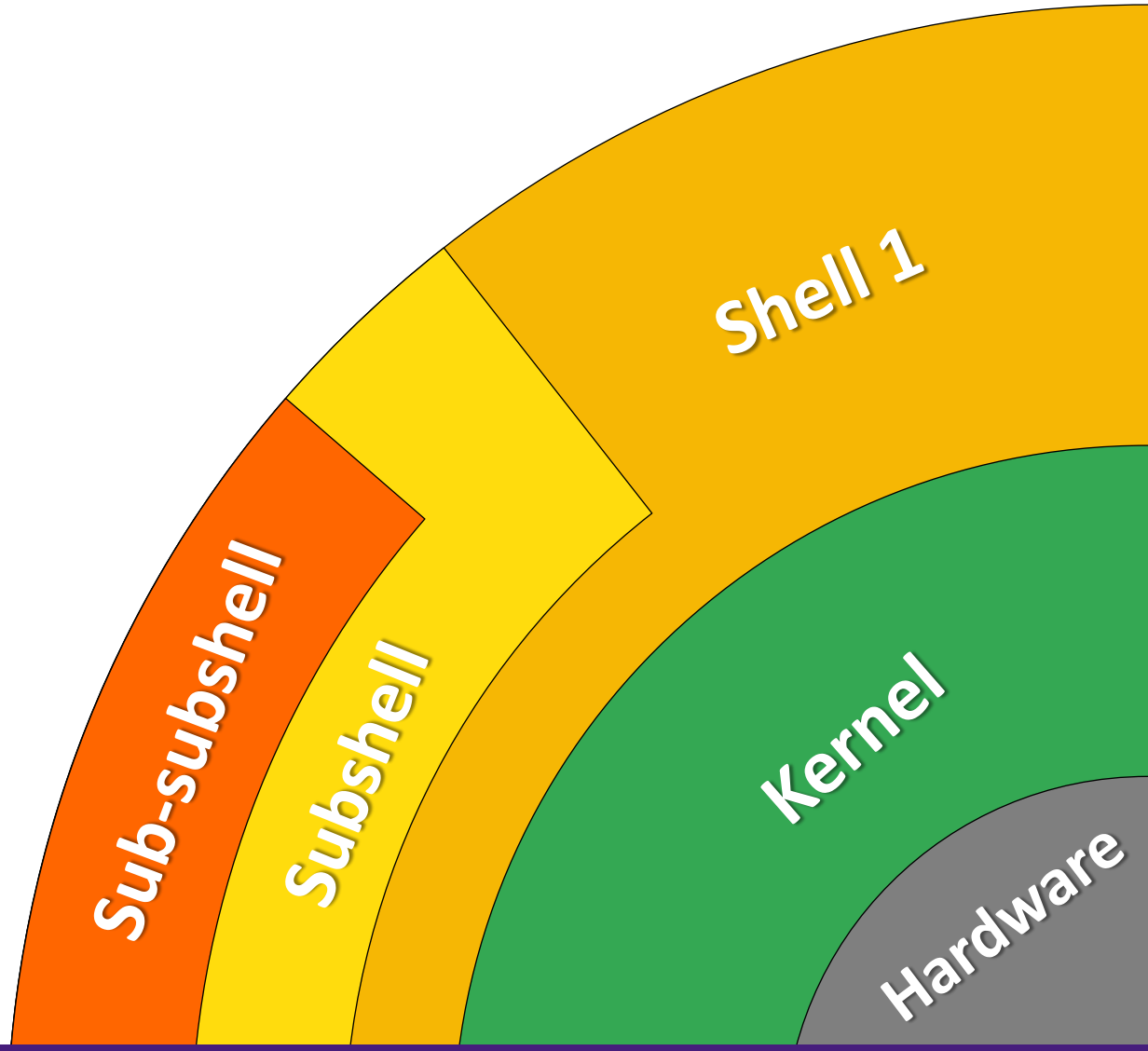
1) Subshells

- **Definition:**
  - A **child process** of launched by an existing shell.
- **Similarity:**
  - **Still a Shell**!
    (Everything we talked about works the same way!)
- **Difference:**
  - An **isolated** environment from its parent
    (A “sandbox” Shell)



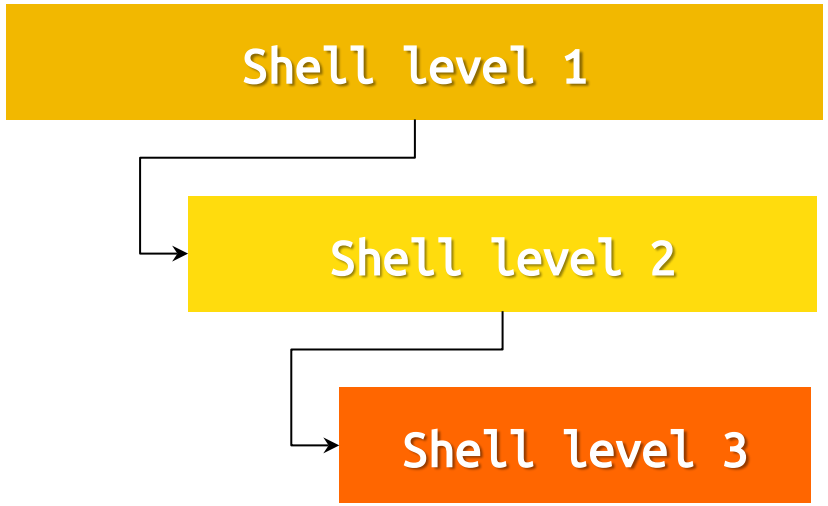
a) Launch a subshell

	Method	Example	Remarks
1	Run a Shell script	`$ ./subshell.sh` `$ bash subshell.sh`	• Can launch **different** Shell types • Check subshell level: `$SHLVL`
2	Explicitly launch an interactive subshell	`$ bash`	
3	Use command grouping "(…)"	`$ (echo "I am in subshell!")`	• Launches the **same** Shell type • Does **NOT** change `$SHLVL`

- What does **NOT** launch a subshell?
  - `source subshell.sh`
  - Commonly used for **environment setting** scripts (You WANT it to set up current Shell)
    - `source setenv.sh`

[1] *ShellScripting/3.1-Subshells/subshell.sh*
[2] *ShellScripting/3.1-Subshells/setenv.sh*

b) Scope of variables



Local variable	Global variable
(Exists only in **current** Shell)	(**Copied** to **all subshells**)
×	×
√	√
×	√

Outlines

2) Flow control

a) Condition – `if` statement

b) Loop – `for` loop

c) Loop – `while` loop

d) Functions

```
#!/bin/bash

# URL and file name
URL=$1
FILENAME=`basename $URL`

# Number of parts
PARTS=$SLURM_NTASKS
echo "Downloading in $PARTS parts..."

# Create temporary directory for parts
TEMP_DIR=$(mktemp -d)

# Calculate the range for each part
FILE_SIZE=$(curl -sIk $URL | awk '/Content-Length/ {print $2}' | tr -d '\r')  # Get file size
PART_SIZE=$((FILE_SIZE / PARTS))  # Calculate part size
LAST_PART_SIZE=$((FILE_SIZE - PART_SIZE * (PARTS - 1)))  # Calculate size of the last part

# Download each part concurrently
for ((i = 0; i < PARTS; i++)); do
  start=$((i * PART_SIZE))
  end=$((start + PART_SIZE - 1))

  if [[ $i -eq $((PARTS - 1)) ]]; then
    end=$((start + LAST_PART_SIZE - 1))
  fi

  curl -ks -o "$TEMP_DIR/part$i" --range "$start-$end" "$URL" &
done

# Wait for all downloads to finish
wait

# Merge the parts into a single file
for ((i = 0; i < PARTS; i++)); do
  cat "$TEMP_DIR/part$i" >> "data/$FILENAME"
done

# Clean up temporary directory
rm -rf "$TEMP_DIR"

echo "Download completed!"
```

a) Condition – `if` statement

- Optional: `elif` and `else`
- **Strict spaces** between "`[ ]`" and conditions
- Use double braces "`[[ ]]`" : More modern features (regular expressions, logic operators, etc.)

Syntax

```
if [ condition ]; then
  # Do something
elif [ condition 2 ] ; then
  # Do something
else
  # Do something else
fi
```

a) Condition – `if` statement

Condition	Syntax
Equal to	`[ $a -eq 0 ] # Integer` `[ $a == $b ] # String`
Not equal to	`[ $a -ne 0 ] # Integer` `[ $a != $b ] # String`
Greater than	`[ $a -gt 0 ] # Integer`
Greater than or equal to	`[ $a -ge 0 ] # Integer`
Less than	`[ $a -lt 0 ] # Integer`
Less than or equal to	`[ $a -le 0 ] # Integer`
Zero length or null	`[ -z $a ] # String`
Non zero length	`[ -n $a] # String`

a) Condition – `if` statement

Condition	Syntax
File exists	`[ -e myfile ]`
File is a regular file	`[ -f myfile]`
File is a directory	`[ -d /home/$USER ]`
File is not zero size	`[ -s myfile ]`
File has read permission	`[ -r myfile ]`
File has write permission	`[ -w myfile ]`
File has execute permission	`[ -x myfile ]`

a) Condition – `if` statement

Condition	`[ ]`	`[[ ]]`
! (NOT)	`[ ! -e myfile ]`	
&& (AND)	`[ -f myfile] && [ -s myfile ]`	`[[ -f myfile && -s myfile ]]`
|| (OR)	`[ -f myfile1] || [ -f myfile2 ]`	`[[ -f myfile1 || -f myfile2 ]]`

- Supported by **more Shells**.
- Use if you need **compatibility**.

- Best supported by **Bash**.
- Use if you need **versatility**.

b) Loop – for loop

– Do something for each element in an array.

Syntax

```
for arg in ${myAry[@]}
do
    # Do something
done
```

b) Loop – for loop

Array	Example

User defined array	`$ myAry=("Alice" "Bob" "Charlie")`
	`$ for arg in ${myAry[@]}`
	…

Shell generated sequence	`$ for arg in `seq 1 4`` …
Output of commands	`$ for arg in `ls $HOME`` …

[1] *ShellScripting/3.2-FlowControl/for.sh*

c) Loop – `while` loop

- Loop as long as `condition` is satisfied.
- Make sure there is an **escape condition** !
  - Otherwise the loop is doomed!

Syntax

```
while [ condition ]
do
    # Do something
done
```

c) Loop – `while` loop

Example

```
$ counter=0
$ while [ $counter -lt 10 ]
do
  echo "Counter is now $counter"
  let counter++    # <- What does this do?
done
```

[1] *ShellScripting/3.2-FlowControl/while.sh*

d) Functions

- A block of pre-defined code that can be reused.
- Passed **arguments** are accessed by:
  - `$1`, `$2`, … `$9`, `${10}`, …
  - `$@` (All arguments)

Syntax

```
# Define
function_name () {
    # Do something
}

# Call, no "()"
function_name [ARG1] [ARG2]
```

d) Functions

Remarks	Example
All variables are **global** by default	`$ myFunc1 () { var="Bob" } $ var="Alice"; myFunc1 ; echo $var Bob`
Local variables must be explicitly declared	`$ myFunc2 () { local var="Bob" } $ var="Alice"; myFunc2 ; echo $var Alice`
Does **NOT** support **return** (Use global variable if needed)	`$ myAdd () { result=$(($1+$2)) } $ myAdd 10 20 ; echo $result 30`

[1] *ShellScripting/3.2-FlowControl/function.sh*

2) Flow control

- **Summary**

a) Condition – `if` statement

b) Loop – `for` loop

c) Loop – `while` loop

d) Functions

Outlines

3) Advanced Text Processing Commands

a) `grep`

b) `sed`

3) Advanced Text Processing Commands

a) `grep`

- **Search** for patterns (formatted strings) in **input stream** (**files** & **pipe**)

Syntax

```
$ grep <options> <search pattern> <files>
```

3) Advanced Text Processing Commands

a) `grep`

i. Basic functionality - Search for a string

Description	Example
Search for lines contain given string in a file	`$ grep "Sales" employee1.txt`
Search for lines do NOT contain given string in a file	`$ grep -v "Sales" employee1.txt`
Search all files for lines contain given string in the directory	`$ grep "Sales" *`
List files that do NOT contain given string in the directory	`$ grep -L "Sales" *`
Search for strings in a pipe	`$ squeue | grep $USER`

[1] *ShellScripting/3.3-TextProcessing/employee1.txt*
[2] *ShellScripting/3.3-TextProcessing/employee2.txt*

a) `grep`

ii. Useful options

Option	Description
`-i`	Ignore cases.
`-r,-R`	Search recursively.
`-v`	Invert match (return those do NOT match pattern)
`-l`	List names of the files that match the pattern.
`-L`	List names of the files that do NOT match the pattern.
`-n`	Print line number with output lines.
…	

[1] https://man7.org/linux/man-pages/man1/grep.1.html

3) Advanced Text Processing Commands

a) `grep`

iii. Pattern

- Can be as simple as strings.
- Can be **Regular Expression** (formatted strings to match beyond fixed strings).

3) Advanced Text Processing Commands

a) grep

iii. Pattern

Metacharacter		Matches	Example
Anchor	^	Beginning of a line.	^Name *(Beginning of a line followed by "Name")*
	$	End of a line.	Salary$ *("Salary" followed by end of a line)*
Substitution	.	Any single character	a.e *(E.g., "age", "ame", "a#e", "a1e",…)*
Repetition	*	Preceding char. repeats **0** or **more** times	50* *(E.g., "5", "50", "500",…)*
	+	Preceding char. repeats **1** or **more** times	50+ *(E.g., "50", "500",…)*
	?	Preceding char. repeats **0** or **1** times	50? *(E.g., "5", "50")*
	{n,m}	Preceding char. repeats **n** to **m** times	50{1,3} *(E.g., "50", "500", "5000")*
Or	[ ]	Any single character inside	[0-9] *(E.g., any single number character)*
	[^]	Any single character NOT inside	[^0-9] *(E.g., any single character but a number)*
	|	Either pattern	Sales|Technology *(E.g., "Sales" or "Technology")*
…			

b) sed

- A powerful “Stream editor” for **text transformation** on input stream (**files** & **pipe**)
- “`grep` searches, `sed` edits”

Syntax

```
$ sed <options> <script> <files>
```

3) Advanced Text Processing Commands

b) sed

i. Basic functionality (all patterns support regular expression)

Function	Usage	Description
Substitution	`$ sed 's/pattern/replacement/flags' file`	For each line, replace matched "pattern" with "replacement", and print out results.
	`$ sed 's/$[0-9]*/$9000/' employee2.txt`	Replace only the first match of each line.
	`$ sed 's/$[0-9]*/$9000/g' employee2.txt`	"Greedy" mode, replace all matches of each line.
Deletion	`$ sed '/pattern/d' file`	Delete lines with matched pattern, and print results.
	`$ sed '/Sales/d' employee2.txt`	Delete all lines matches "Sales".
	`$ sed '2,4d' employee2.txt`	Remove line 2 through 4.
Insertion	`$ sed '/pattern/ i\newline' file  # Insert before` `$ sed '/pattern/ a\newline' file  # Insert after`	Insert / Append new line at specific location, and print results.
	`$ sed '/Alice/ i\newline'`	Insert before lines matches "Alice".
	`$ sed '3 a\newline'`	Append to line 3.
…		

[1] *ShellScripting/3.3-TextProcessing/employee2.txt*

b) sed

ii. Other common usage

Usage	Example	Description
`$ sed -i <script> file`	`$ sed -i 's/$[0-9]*/$9000/' employee2.txt`	Change file **in-place** instead of printing results.
`$ sed -e <script1> -e <script2> file`	`$ sed -e 's/$[0-9]*/$9000/' \` `  -e 's/Rep/Assistant/' employee2.txt`	Execute **multiple** scripts.
`$ cmd | sed <options> <script>`	`$ conda env list | sed '/^#/d'`	Parsing **piped output** instead of file.

[1] *ShellScripting/3.3-TextProcessing/employee2.txt*

3) Advanced Text Processing Commands

- **Summary**
  - "`grep` searches, `sed` edits."

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4. **BONUS: Where to Get Help**

BONUS: Where to Get Help

- **I need more help with Shell scripting. Where do I get help?**

1) Contact HPC User Services

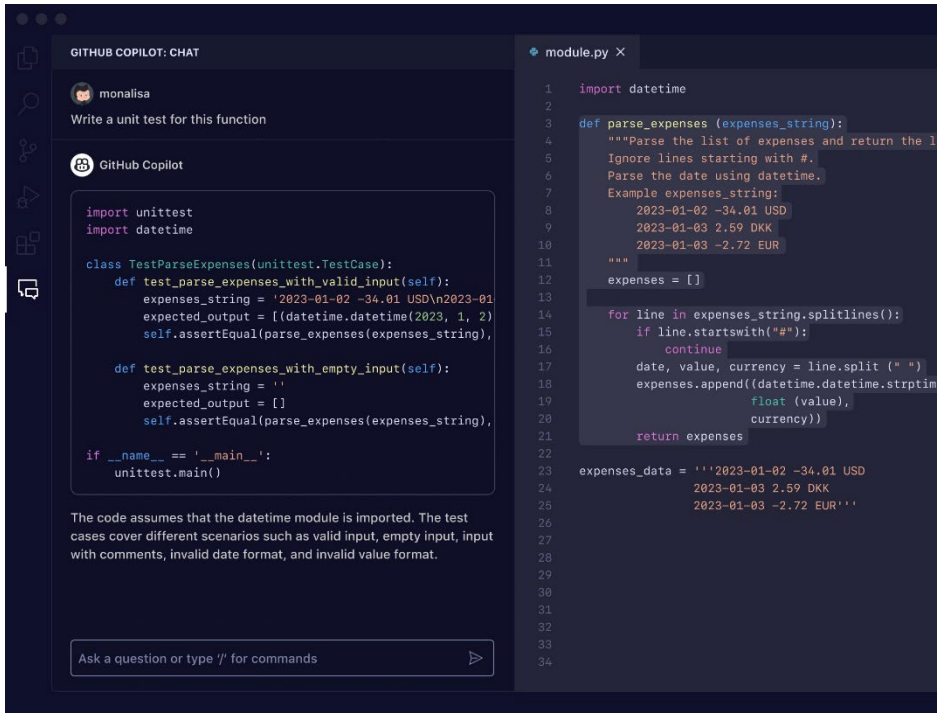
  - Email Help Ticket: sys-help@loni.org
  - Telephone Help Desk: +1 (225) 578-0900

BONUS: Where to Get Help

- **I need more help with Shell scripting. Where do I get help?**

2) Generative AI

ChatGPT



GitHub Copilot

BONUS: Where to Get Help

- **Why I recommend generative AI for Shell scripting?**

Shell scripting

- Something you may not be too familiar with, but have to work with on a daily basis for HPC jobs.
- A **quick and dirty** solution for automation. Not comprehensive software framework.
- Usually just need to **get the job done**. Do not care for reliable sources (unlike doing research).

Generative AI

- Easy to get an answer without extensive knowledge.
- Good at **giving quick and dirty answers**. Not suitable for building comprehensive software framework.
- **Experienced, but not scientific**. Trained with collective human knowledge pool. But bad at selecting particular reliable sources.

BONUS: Where to Get Help

- **Steps**

1) Find out what you want to do and ask AI the right questions

- Try these examples (think about how to do it first, then ask AI):

a) Change all text "`/ddnB/work`" to "`/work`" in all files in folder "`~/mycode/`" and subfolders.

b) In a "`,`" separated .csv database, delete all columns starting from the 10th, and add an index column as the first column.

c) Run executable "`myexec`" with "`input.txt`" as standard input, but replacing all "`TIME`" text in "`input.txt`" with current timestamp generated by "`date`".

BONUS: Where to Get Help

- **Steps**

  2) **TEST! TEST! TEST!**

    - AI generated scripts may not work right away!
    - Test it in a **safe** & **isolated** environment (a sandbox) first, especially your script is something destructive!
    - You may need to come back and ask AI to revise your script.

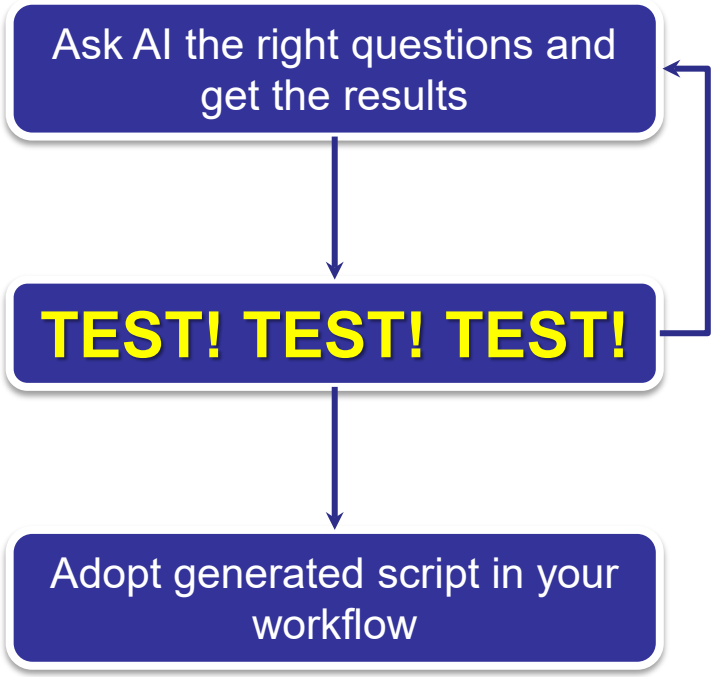
BONUS: Where to Get Help

- **Steps**

  3) Adopt in your workflow

BONUS: Where to Get Help

- **Steps**



Conclusion

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4. **BONUS: Where to Get Help**

Conclusion

- **Take-home message:**

When NOT to use Shell scripting?

- Heavy calculation!

When to use Shell scripting?

- Automating job workflow
- Pre-processing / Post-processing
- …

Contact us

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