# 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

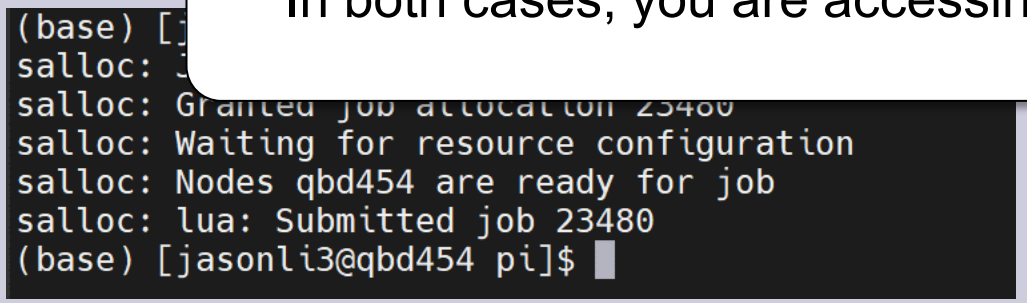
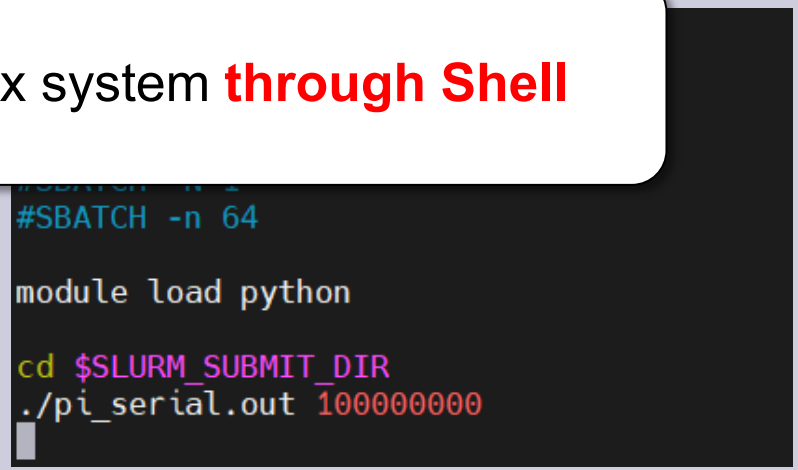
- **Example and exercises:**
  - http://www.hpc.lsu.edu/training/weekly-materials/Downloads/ShellScripting.zip

# 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**

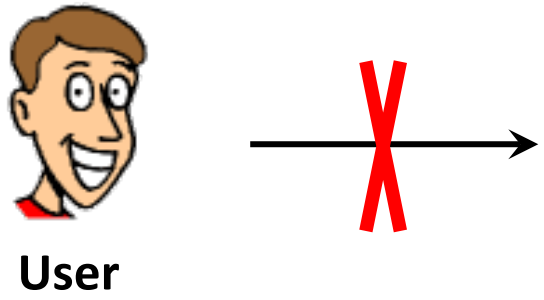
# 1) What's Shell?

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

| 1) Interactive job | 2) Batch job |
| --- | --- |
|  |  |

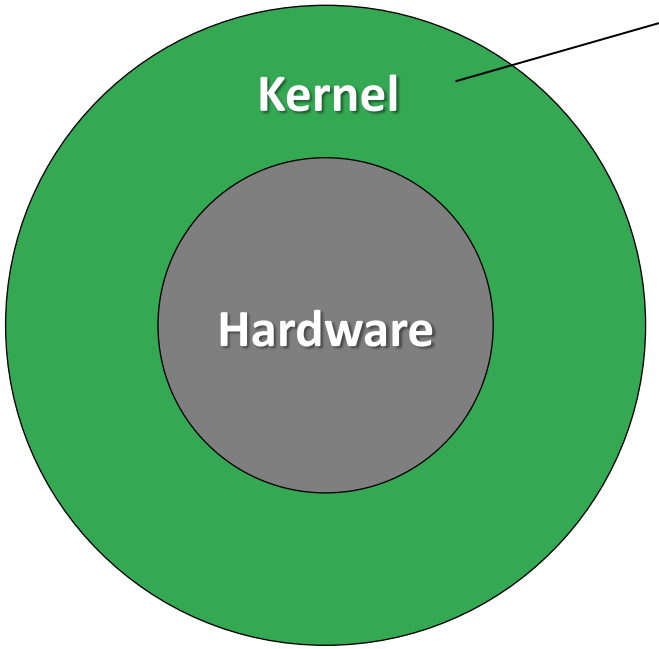
In both cases, you are accessing a Linux system **through Shell**

# 1) What's Shell?



User



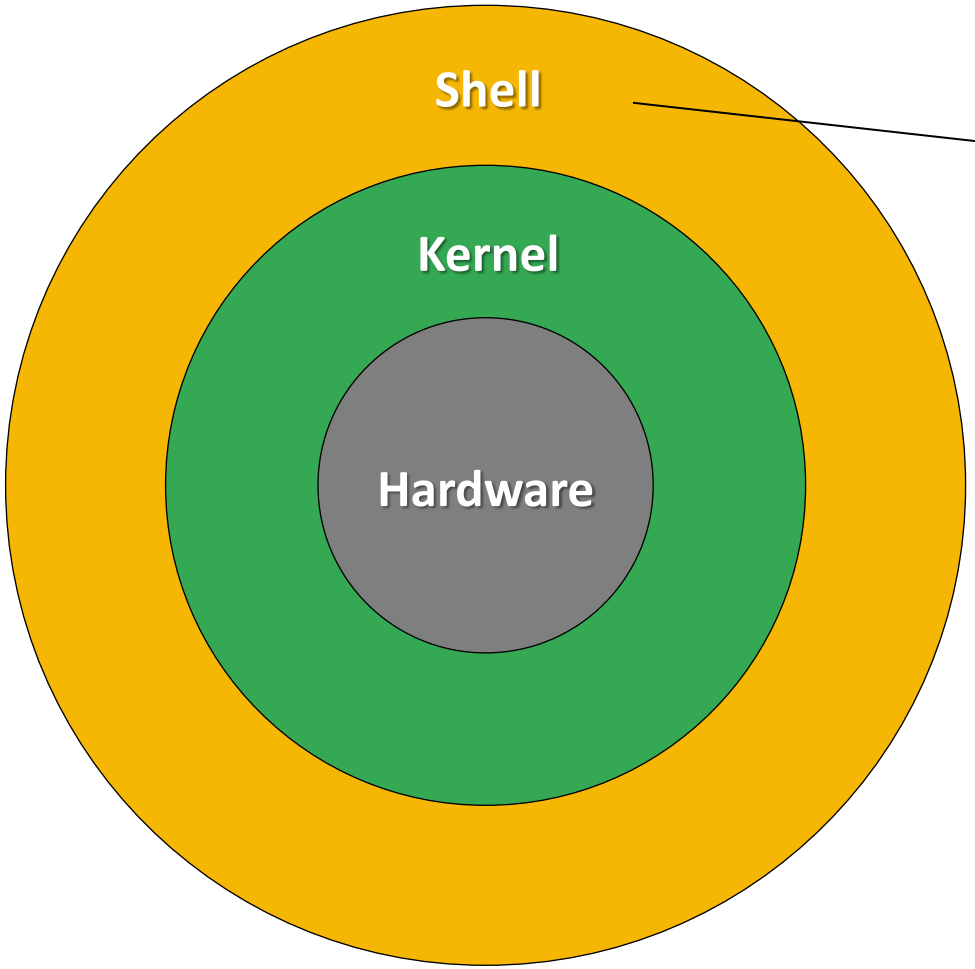



- Resource management
- Process management
- Device Drivers
- System Calls
- …

→ **Speaks: Machine**

# 1) What's Shell?

User

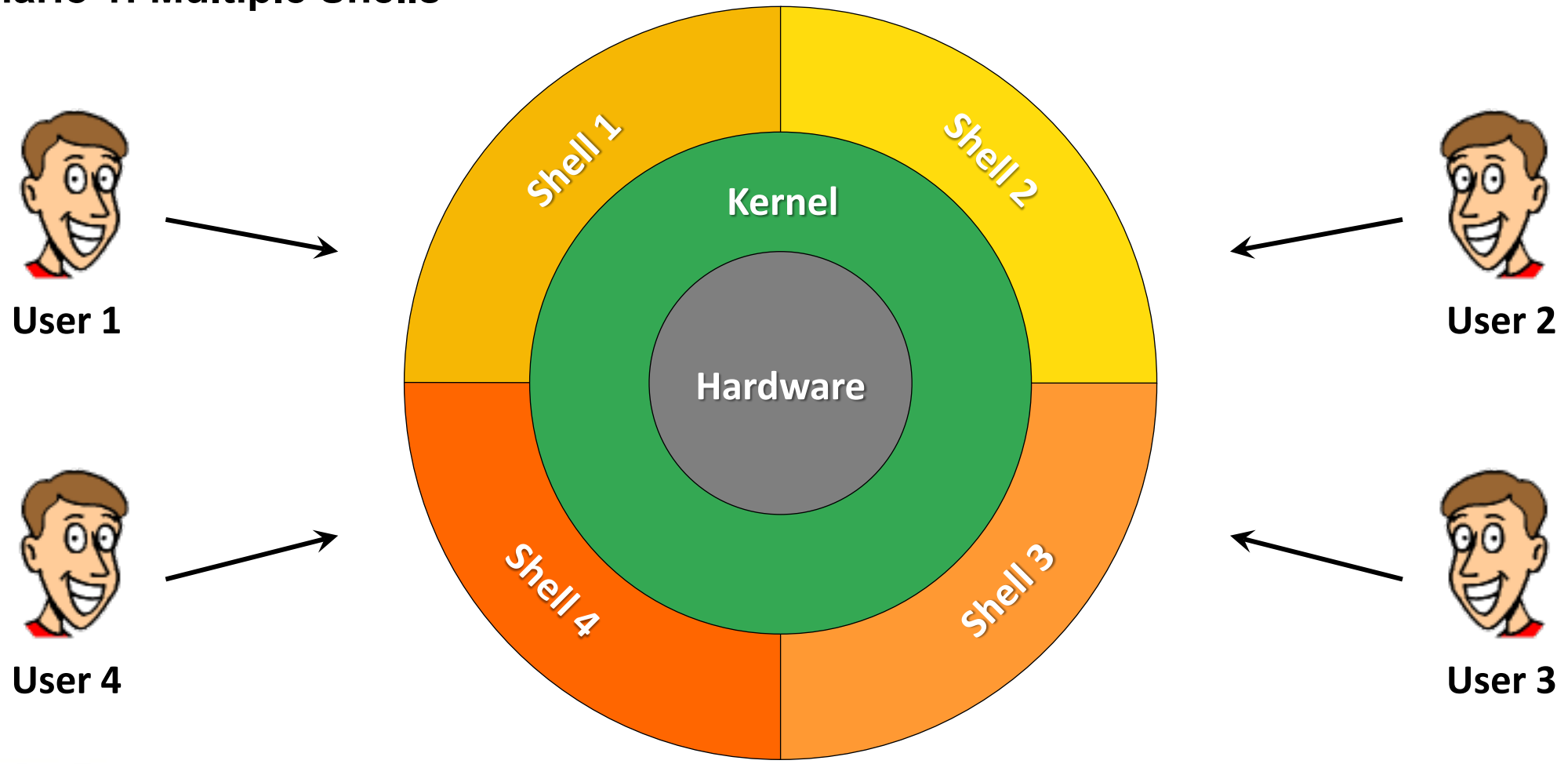



- Command execution
- Scripting
- …

→ **Speaks: Human**

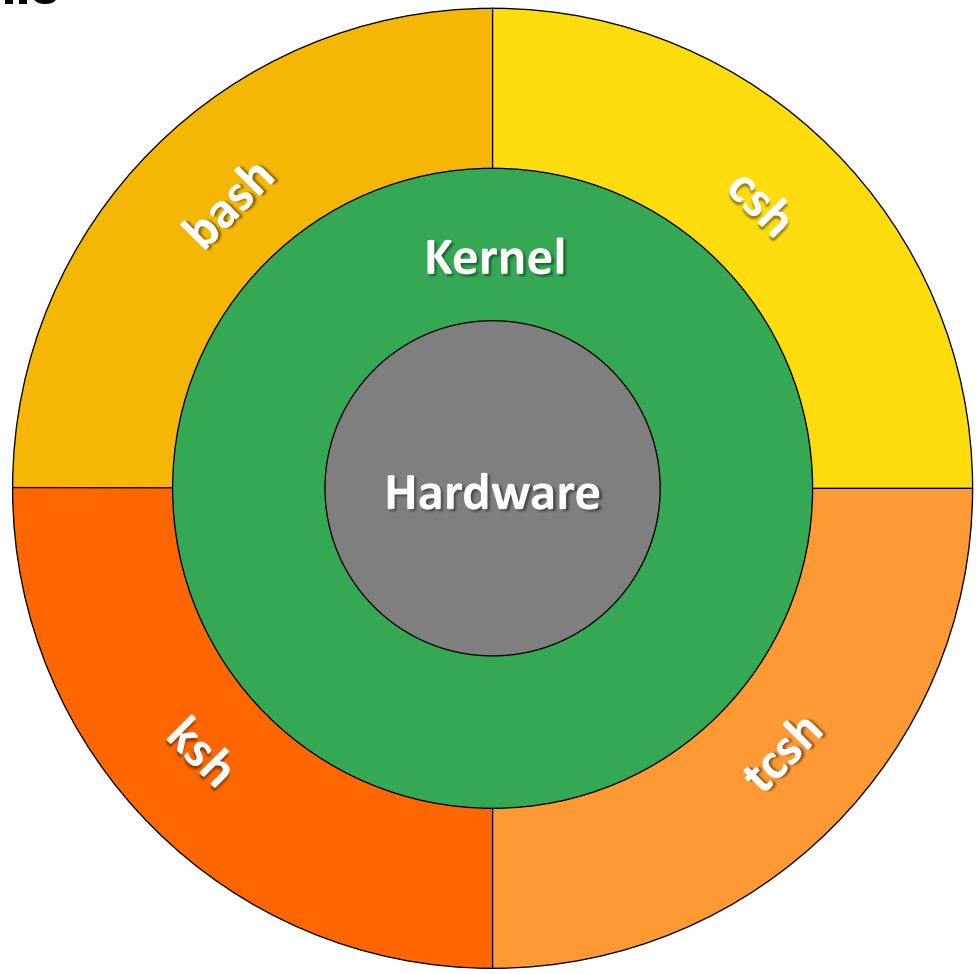
# 1) What's Shell?

- **Scenario 1: Multiple Shells**



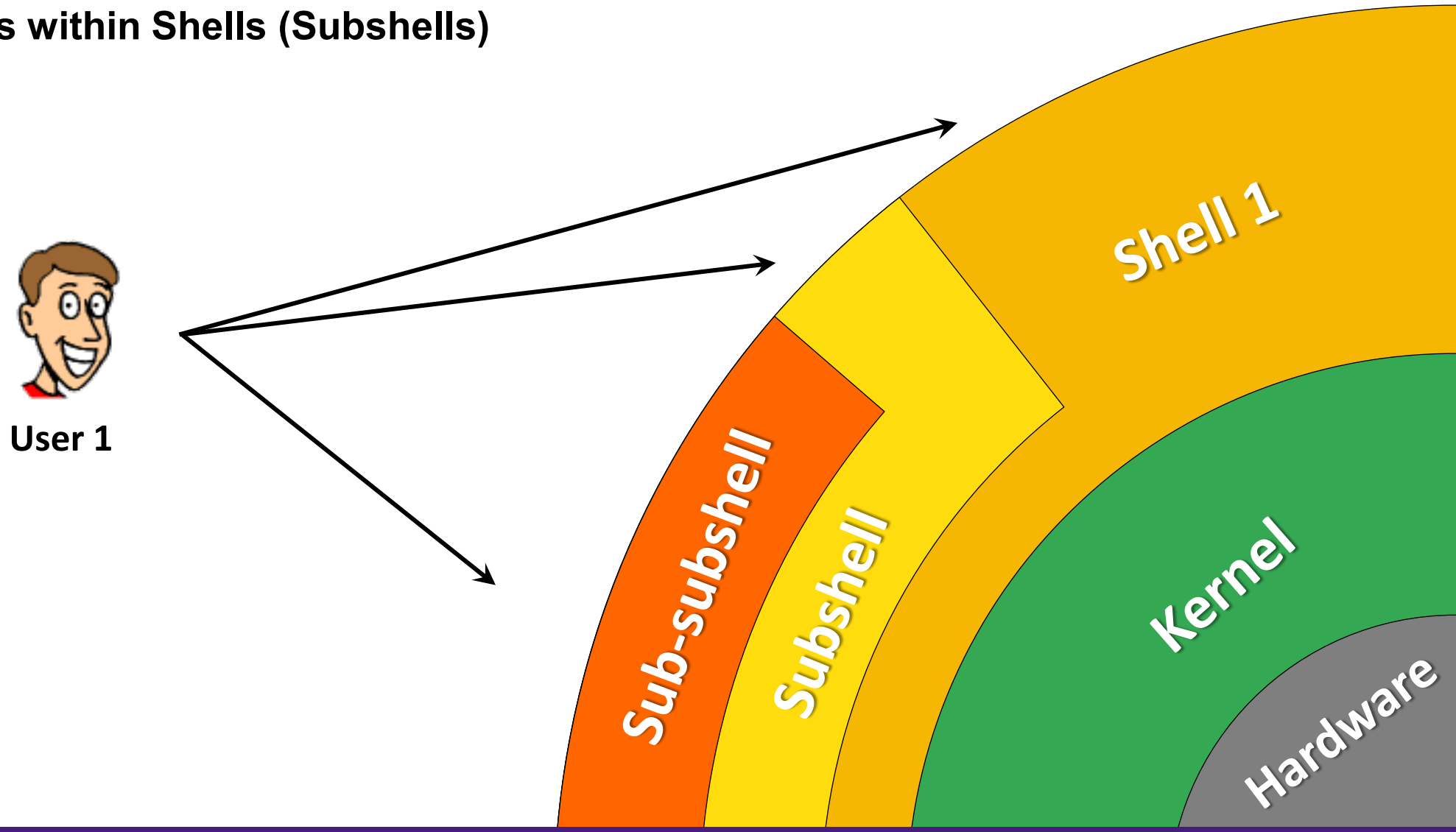
# 1) What's Shell?

- **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 $SHELL
/bin/bash
(base) [jasonli3@qbd1 ShellScripting]$ cd exec
(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
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# 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:**

```bash
#!/bin/bash

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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:**

| Why would I need … | If I can just use … |
|---|---|
| Shell | Another language (Python / C++ / Fortran) |
| Another language (Python / C++ / Fortran) | Shell |

# 2) What can Shell do?

## a) Why would I need Shell if I can just use 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*

# 2) What can Shell do?

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

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

# 2) What can Shell do?

- **Rule of thumb:**

**Anything you wish to run faster, you should NOT use shell!**

# 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!)<br>• Replacing your known language / software | • **Automating job workflow** with minimum scripting (e.g., set up environment, call proper executables, etc.)<br>• **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**.<br>• Able to use Shell scripting to **optimize job workflow**. |

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   2) What can Shell do?
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   2) Basic Commands & Syntax
   3) Variables
   4) Arrays
   5) Arithmetic Operations
3. Beyond Basics
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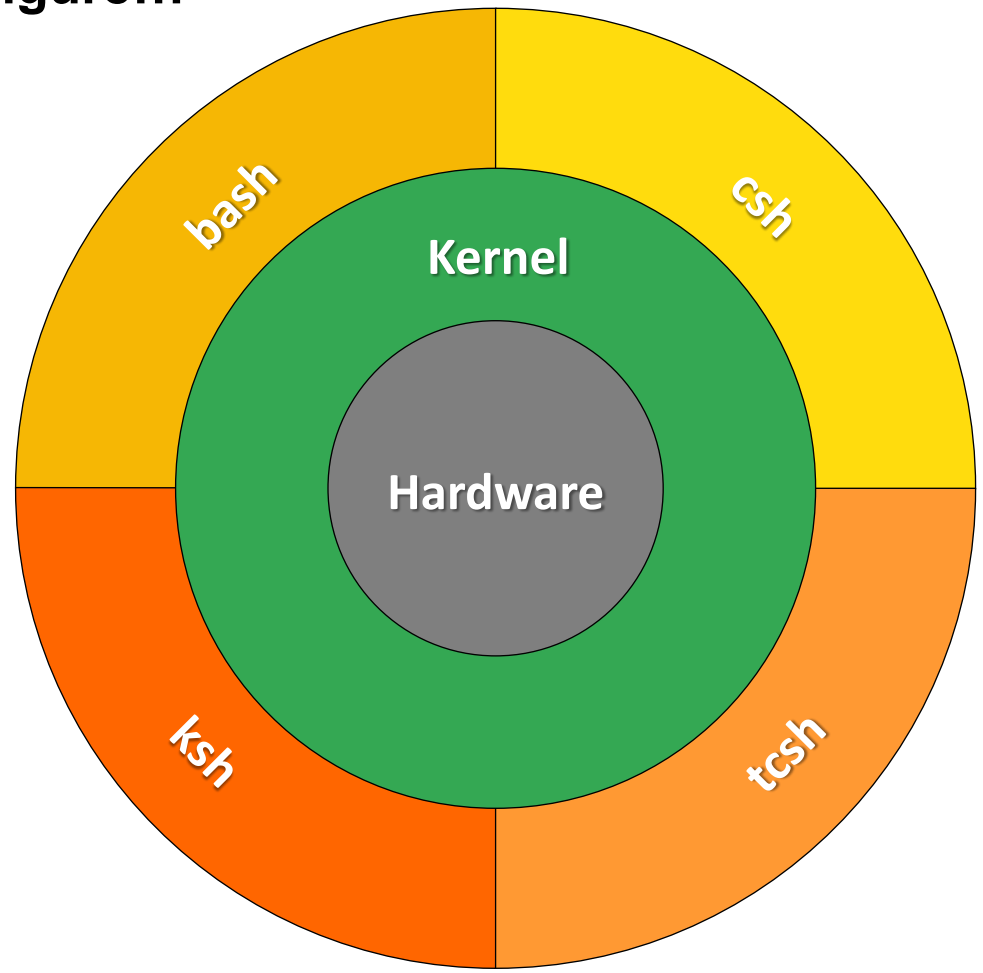
# Before we continue…

- **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)
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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]$ 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]$
```

### Non-interactive

```
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FILENAME=`basename $URL`

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  end=$((start + PART_SIZE - 1))
```

# 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
URL=$1
FILENAME=`basename $URL`

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

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# 1) Interactive vs Non-interactive Shell

## a) Two ways to access Shell

### Interactive

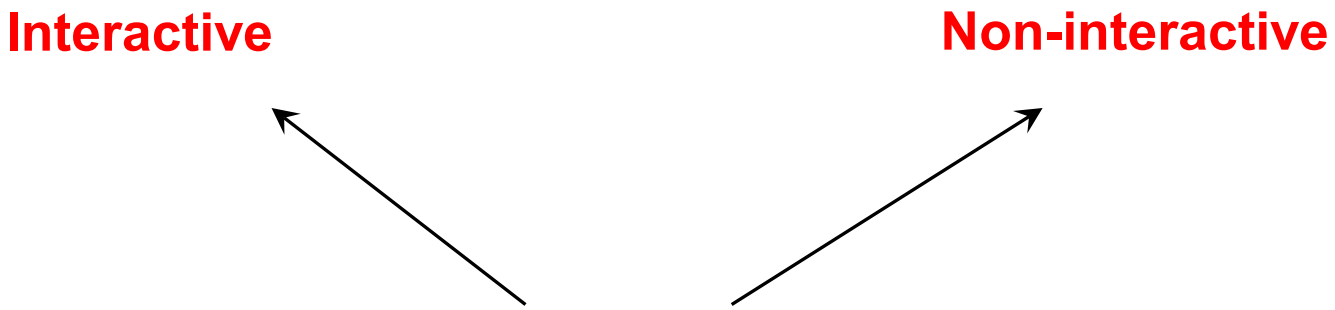
- Runs in terminal
- Can interact in real time
- Type commands one-by-one
- E.g., every time you log in in terminal

### 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

" ***Shebang*** " -

- Shell to run this script with

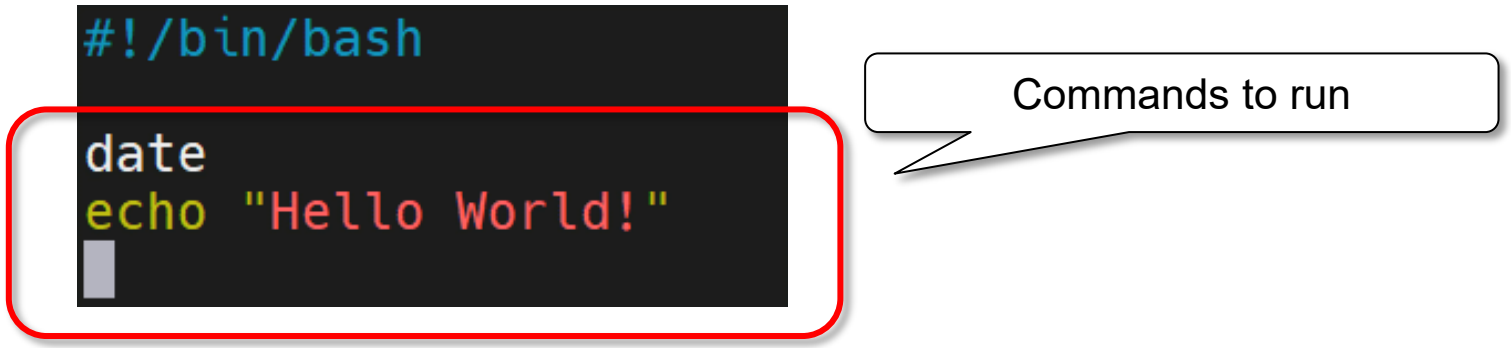
```
#!/bin/bash

date
echo "Hello World!"
```

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

# 1) Interactive vs Non-interactive Shell

## 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 | | | |
|---|---|---|---|---|---|---|
| | | | Must be executable? | Which Shell? | Start subshell? | Others |
| 1 | Use **full path** (Most common) | `$ ./helloworld.sh`<br>`$ /path/to/helloworld.sh` | √ | **Shebang** (if exist) or **default** Shell | √ | - |
| 2 | Use **specific Shell** | `$ bash helloworld.sh`<br>`$ csh helloworld.sh` | × | **Specified** Shell | √ | - |
| 3 | Use "**source**" or "**.**" | `$ source helloworld.sh`<br>`$ . helloworld.sh` | × | **Current** Shell | × | - |
| 4 | Run as **Shell command** | `$ helloworld.sh` | √ | **Shebang** (if exist) or **default** Shell | √ | Parent directory must be included in **$PATH** environment variable |

Run "`chmod u+x [filename]`" if file is not executable

[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`<br>`$ ./testoutput 1> out.txt 2> err.txt` |
| >> | **Redirect (Output)**: Redirect standard output / error to file. This method appends to the file. | `$ ./testoutput >> out.txt`<br>`$ ./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. | `$ sleep 10 &` |

[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
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   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 $workdir` | |
| | `$ mycmd="/home/jasonli3/myexec"`<br>`$ myout="/work/jasonli3/out.txt"` | `$ $mycmd > $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**:

- 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. |
| | SHELL | Default Shell |
| | **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 $USER"`<br>`echo jasonli3` |
| '' | Preserves the literal value of **ALL CHARACTERS** within the quotes. | `$ echo 'echo $USER'`<br>`echo $USER` |
| `` | **Command substitute**: Execute the command(s) inside the quotation and use its output to replace the quotation. | `$ echo `echo $USER``<br>`jasonli3` |

# Outlines

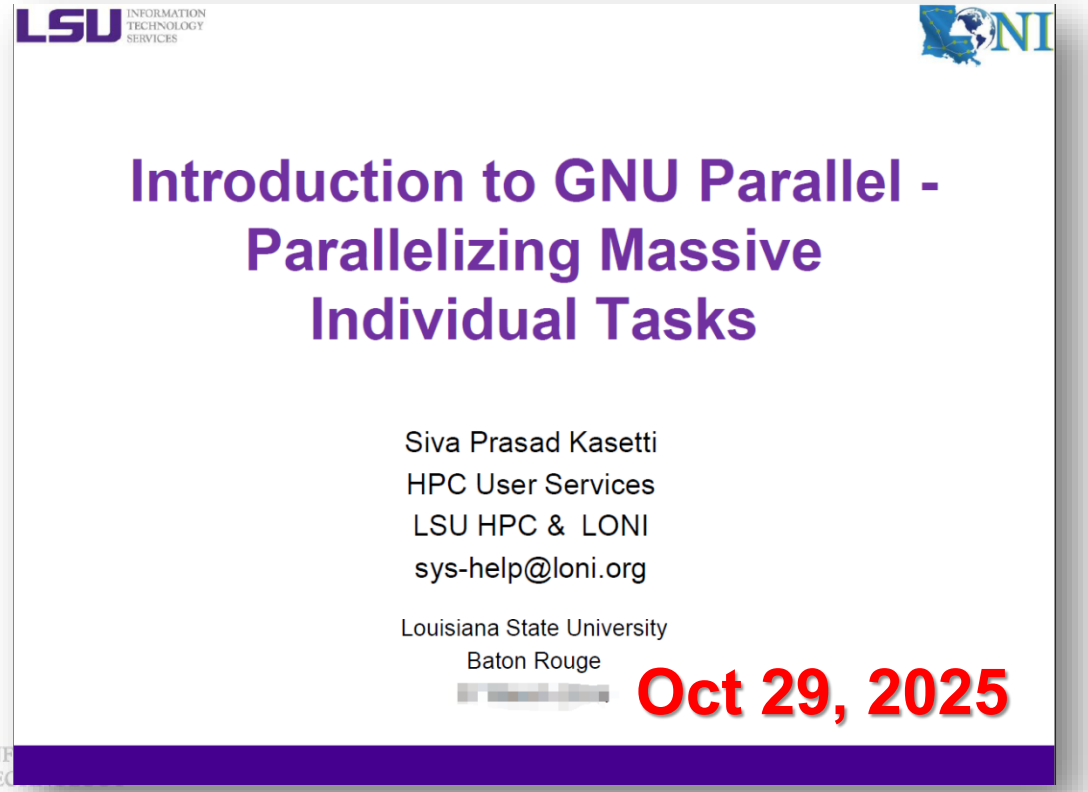
# 4) Arrays

- **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?



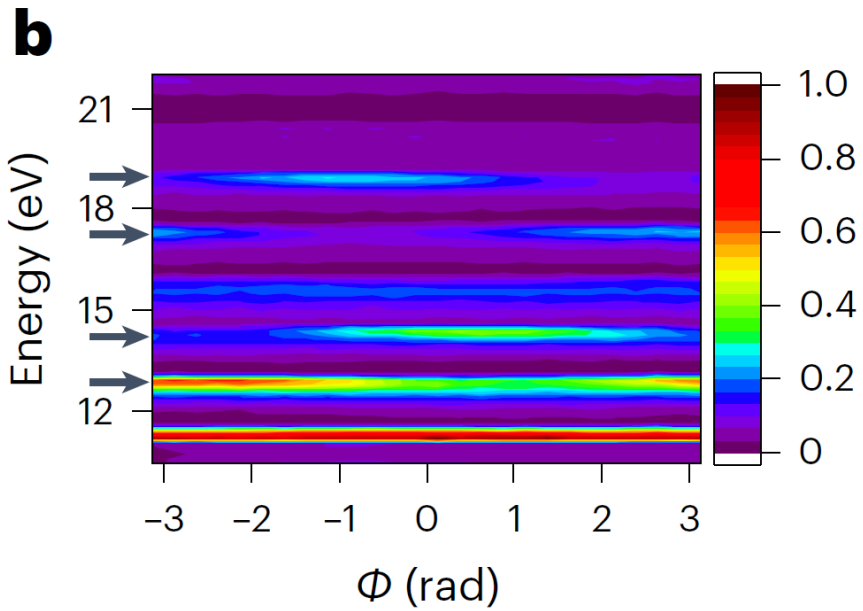

```
$  parallel myexec ::: ${inputParams[@]}
```

[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.<br>• **Integers** only! |
| 2 | `let` (Slightly more advanced) | `$ let b=$a/3+2`<br>`$ let b=a/3+2`<br>`$ let b++` | • Evaluate **assignment** w/ arithmetic calculation.<br>• "`$`" can be emitted.<br>• **Integers** only! |
| 3 | `expr` (Legacy, most limited) | `$ expr $a / 3 + 2` | • Strictly limited to "`ARG1 OPERATION ARG2`" format.<br>• **Integers** only! |
| 4 | `bc` (Most powerful) | `$ bc`<br>`scale=3`<br>`a=10;a/3+2`<br>`$ bc < bcExample.txt`<br>`$ echo "$a/2+3" \| bc` | • **Interactive** and **non-interactive** mode.<br>• Does **NOT** support Shell syntax (namely, "`$`" for variables).<br>• Unassigned variables treated as `0`.<br>• `scale` variable determines number of decimals.<br>• 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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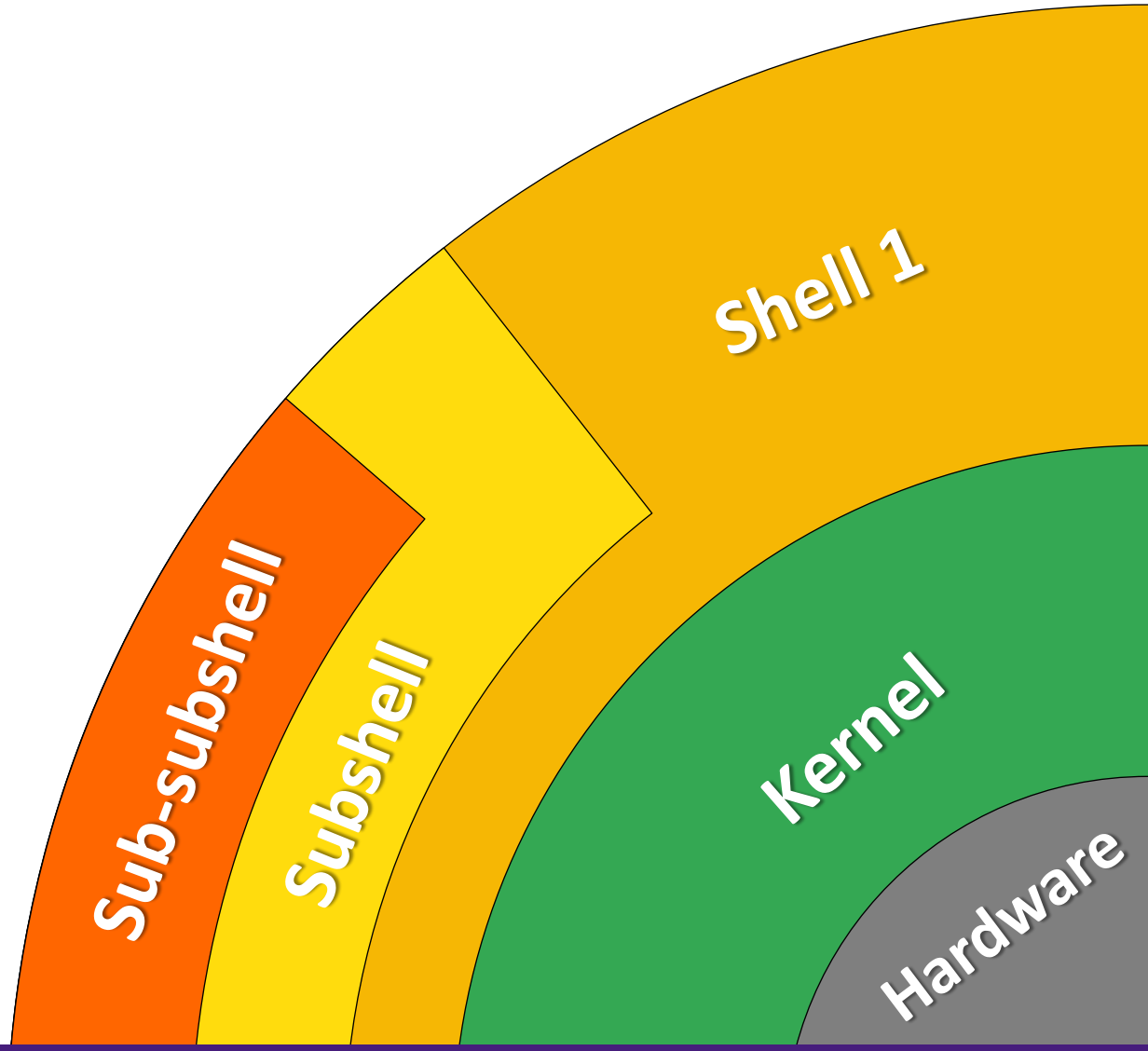
# 1) Subshells

- **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)



# 1) Subshells

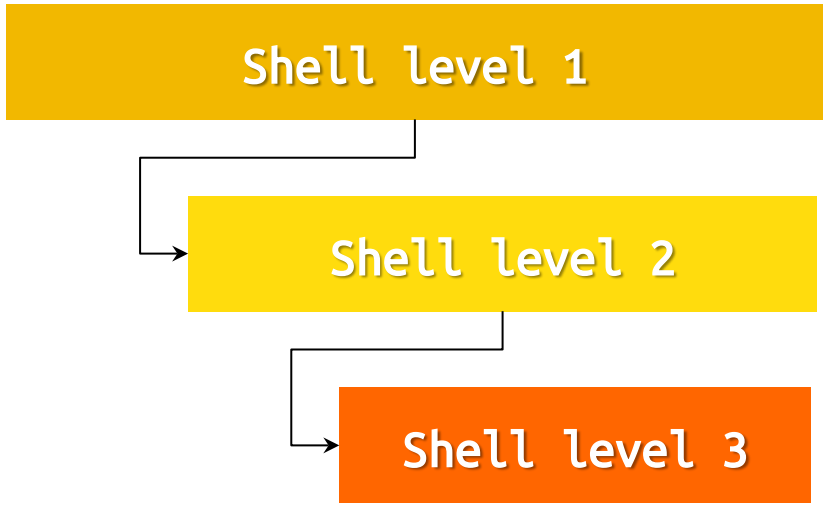
## a) Launch a subshell

| | Method | Example | Remarks |
|---|---|---|---|
| 1 | Run a Shell script | `$ ./subshell.sh`<br>`$ bash subshell.sh` | • Can launch **different** Shell types<br>• 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<br>• 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**) |
| Shell level 1 | × | × |
| Shell level 2 | √ | √ |
| Shell level 3 | × | √ |

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# 2) Flow control

a) Condition – `if` statement

b) Loop – `for` loop

c) Loop – `while` loop

d) Functions

```bash
#!/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`<br>`[ $a == $b ] # String` |
| Not equal to | `[ $a -ne 0 ] # Integer`<br>`[ $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")`<br>`$ for arg in ${myAry[@]}`<br>… |
| Shell generated sequence | `$ for arg in `seq 1 4``<br>… |
| Output of commands | `$ for arg in `ls $HOME``<br>… |

[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` → search

b) `sed` → edit

# 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*

# 3) Advanced Text Processing Commands

## 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

## 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**)

**Syntax**

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

## 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`<br>`$ 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*

# 3) Advanced Text Processing Commands

## 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]*/$9000/' \`<br>`  -e 's/Rep/Assistant/' employee2.txt` | Execute **multiple** scripts. |
| `$ 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

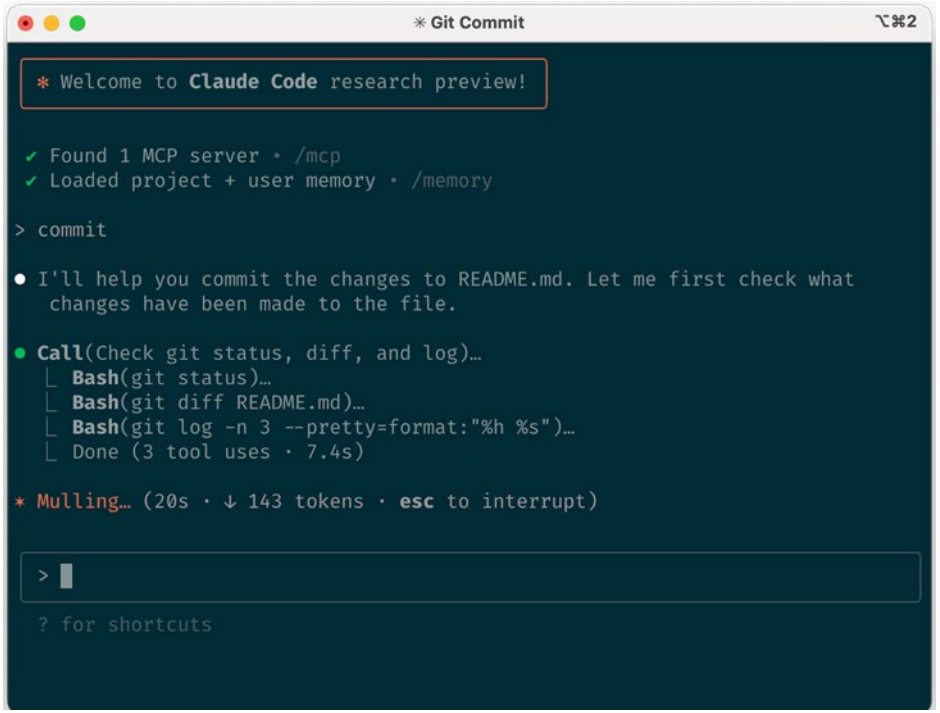
  - Email Help Ticket: sys-help@loni.org
  - Telephone Help Desk: +1 (225) 578-0900

# BONUS: Where to Get Help

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

## 2) Generative AI


ChatGPT

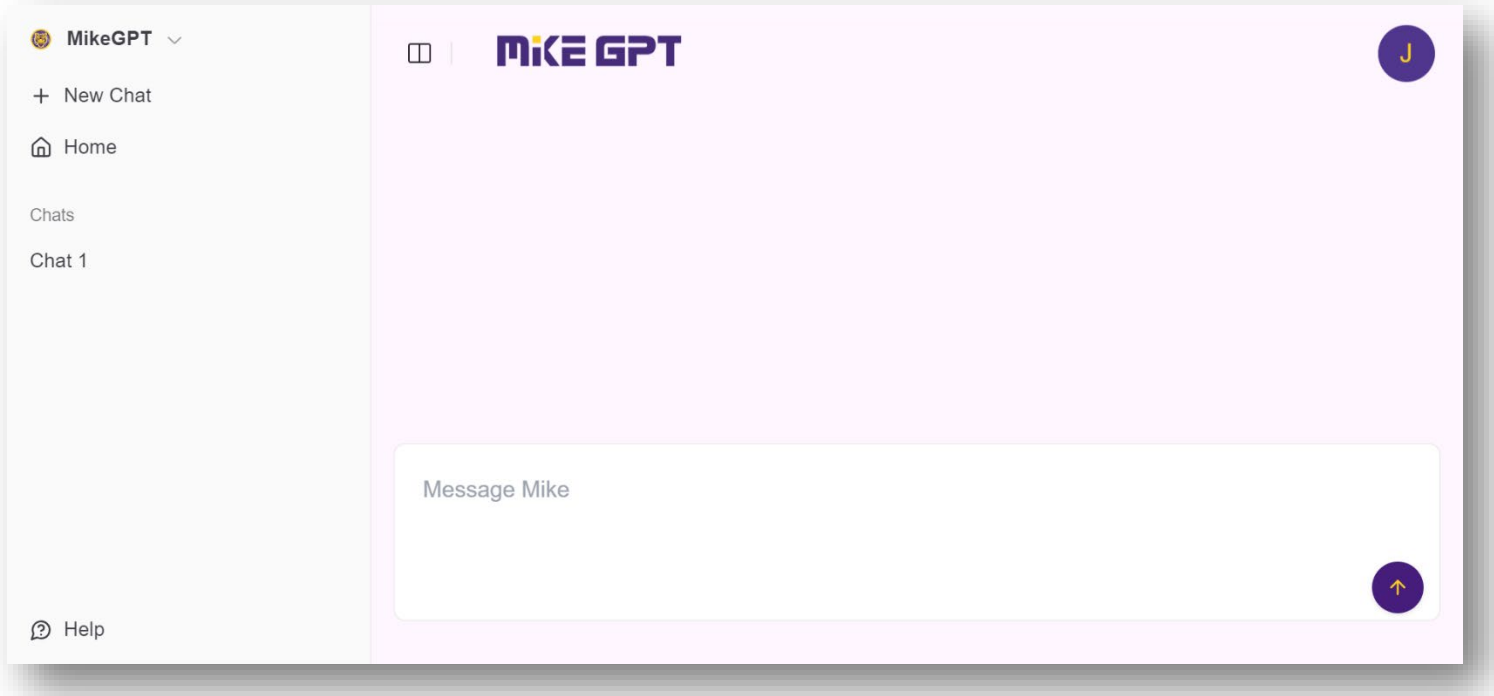



Claude Code

# BONUS: Where to Get Help

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

**2) Generative AI**




**MikeGPT**

(LSU's own GPT chat box! Trained with LSU public realm data)

[1] https://mikegpt.lsu.edu/

# BONUS: Where to Get Help

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

| Generative AI | Shell scripting |
| --- | --- |
| • Good at giving **quick and dirty answers**.<br>• Bad at giving **reliable sources**. | • **Quick and dirty** answer is all you need!<br>• Don't really care about sources. |
| • Good at coding.<br>• Bad when code is too long & complicated. | • **One line** is all you need |

# 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.

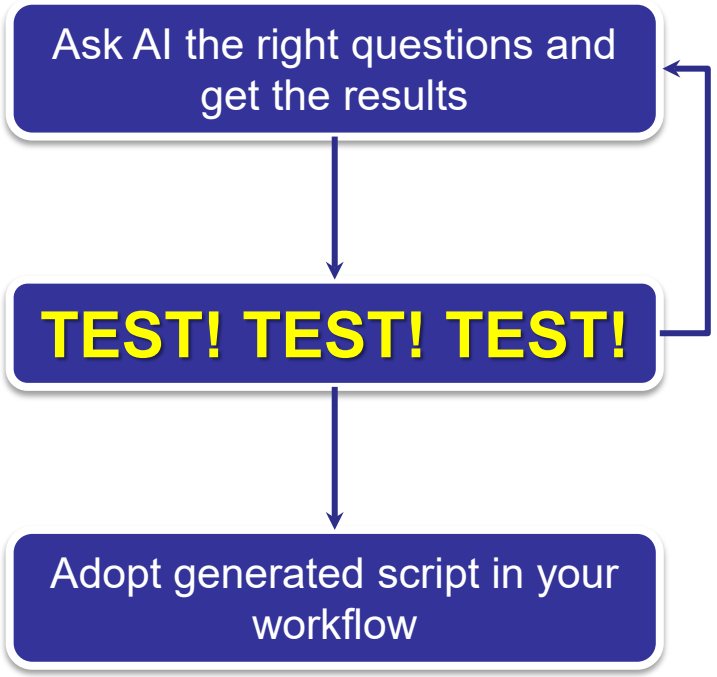
# BONUS: Where to Get Help

- **Steps**

  3) Adopt in your workflow

# BONUS: Where to Get Help

- **Steps**



# Conclusion

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**

# Conclusion

- Take-home message:

**Anything you wish to run faster, you should not use shell!**

**When NOT to use Shell scripting?**

- Heavy calculation!

**When TO use Shell scripting?**

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

# Contact us

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