UCSB, Physics 129AL, Computational Physics: Problem Set 1

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Due: Jan 21, 11:59PM

Problem Set Submission Guideline

A) Github Submissions We will use GitHub for problem set submissions. To access the problem set, please **fork** and **clone** the **forked** repository to your local virtual machine. **Please complete the problem set in this forked directory.** Submit **a pull request** for merging into the main branch before the problem set due date.

B) Export Command History: Please submit all of your commands (including errors) in a text file named "history.txt" in the problem set directory. For instance, to select and append the last 10 commands to the file, use the following history command: "history | tail -n 10 >> history.txt". Note that the last command in the text file will be the history command mentioned above.

C) .tar.gz File compression and submission on Github for each problem set, you are asked to submit the compress version of the problem set to github via git operation. Here is a step by step guideline,

1. Use the **tar** command to compress the problem set directory into a **single** ".tar.gz" file.
2. Obtain the sha256sum by running "sha256sum #.tar.gz" (#: problem set number).
3. Echo the **full sha256sum** to a text file named "sha25sum_problem_set.txt".
4. Initialize a git repository named"Archive_P# (#: problem set number) on your local machine, and move both the "tar.gz" file and the "sha25sum_problem_set.txt" file to the repository.
5. Create an empty **public** directory udner the **same name** in **your own github account**.
6. **Push** this local repository to the remote repository.

In summary, by the end of the due date, you should have two directories: one is the **forked directory, where you submit your pull request**, and the

other is **your own archive directory**. In this problem set, you are asked to follow the above guideline, otherwise, you will receive zero for the problem set.

I put some notes for references, and the problem set starts with "Problem #". **Remember, talk to your fellow students and work together. You will find it much easier than working alone. Good luck!**

1 Basic Bash command usages

First created in Bell Labs in the late 1960s and early 1970s, UNIX treats everything as a file where it can be managed in a unified manner. It offers a rich set of commandline tools for performing file operations. We will look at a few basics commands in Linux here. Fig.1: we explore few basic commands in Linux file management, e.g. "mkdir", "ls", "cd", "echo", "cat", "¿,¿¿". Fig.2: "ls -l" command lists all files and their properties. The total is usually used to estimate the disk usage of a given directory. Fig.3: Standard input, output, and error. Fig.4: Grep keywords in a file. Fig.5: Find files and execute commands. Fig.6: Pipelines. Fig.7: General commands, e.g. "touch", "mv", "rm", "cp", "chmod", "ln -s", "alias", and "unalias". Fig.8: Archives and Tar format.

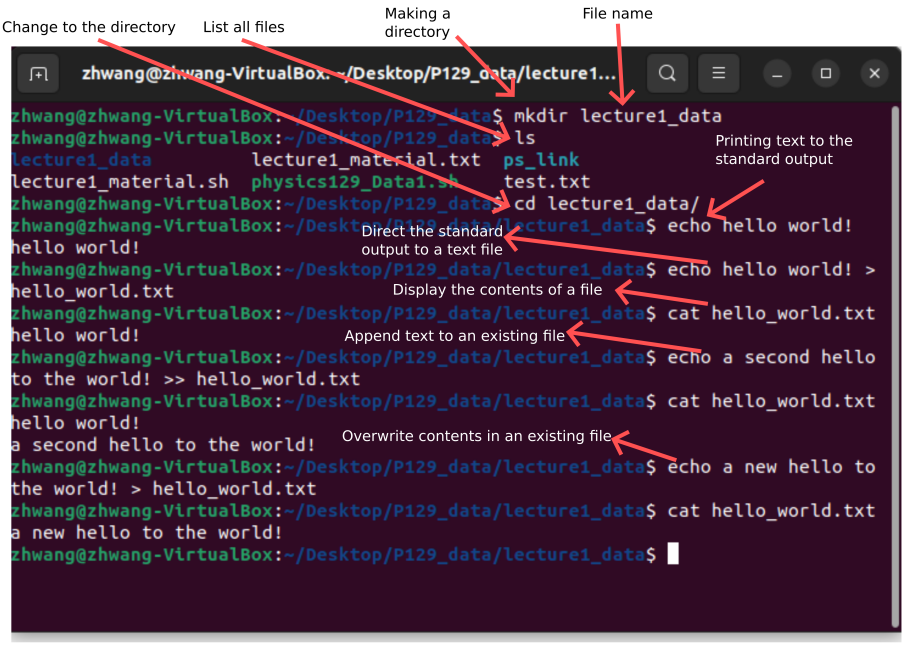


Figure 1: basic commands.

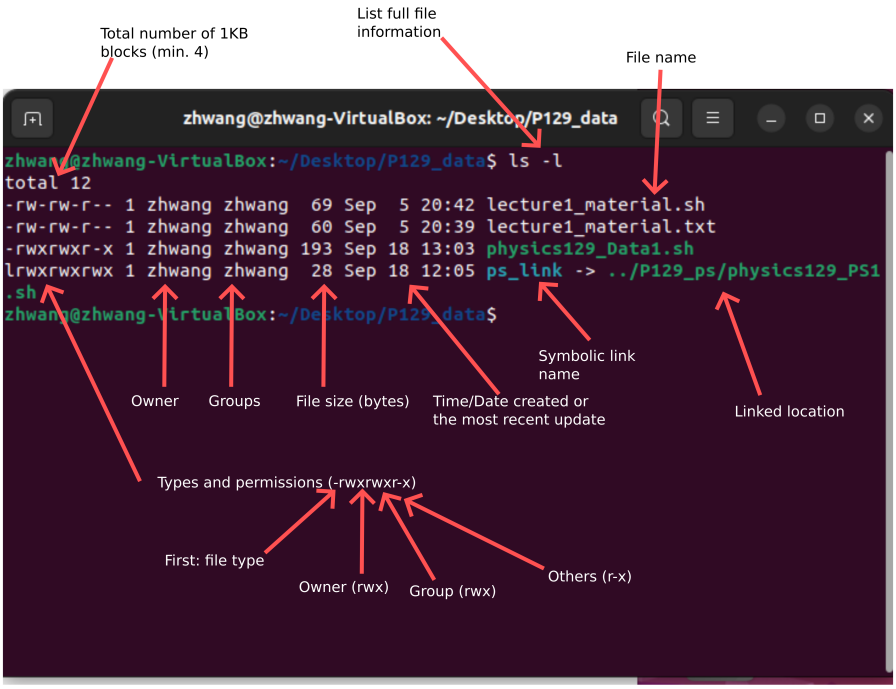


Figure 2: "ls -l" command.

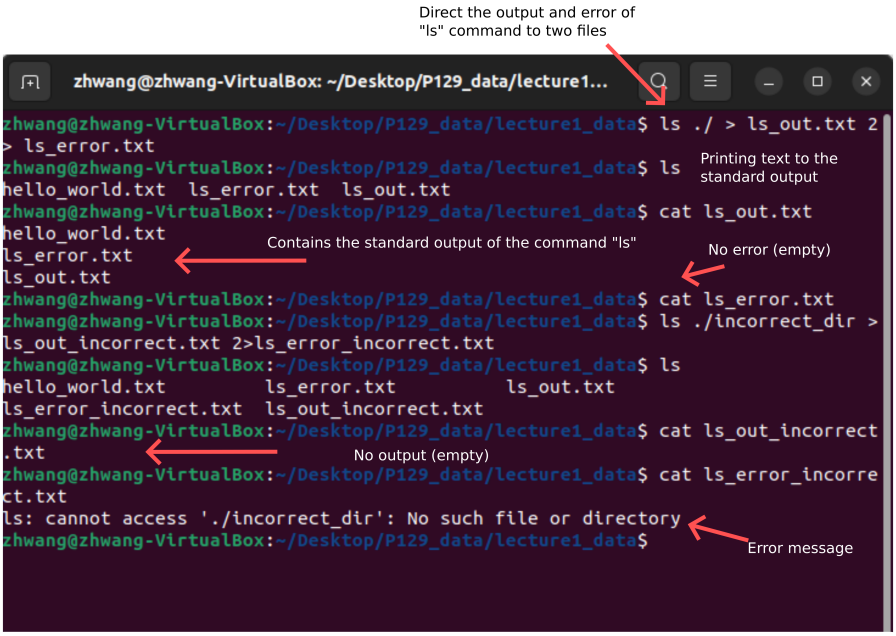


Figure 3: Standard input, output and error.

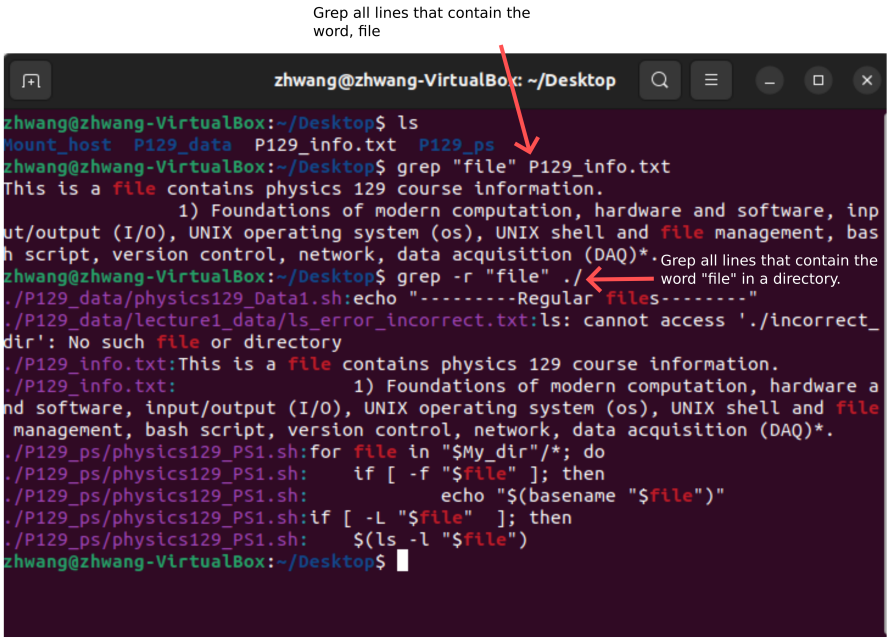


Figure 4: Grep keywords.

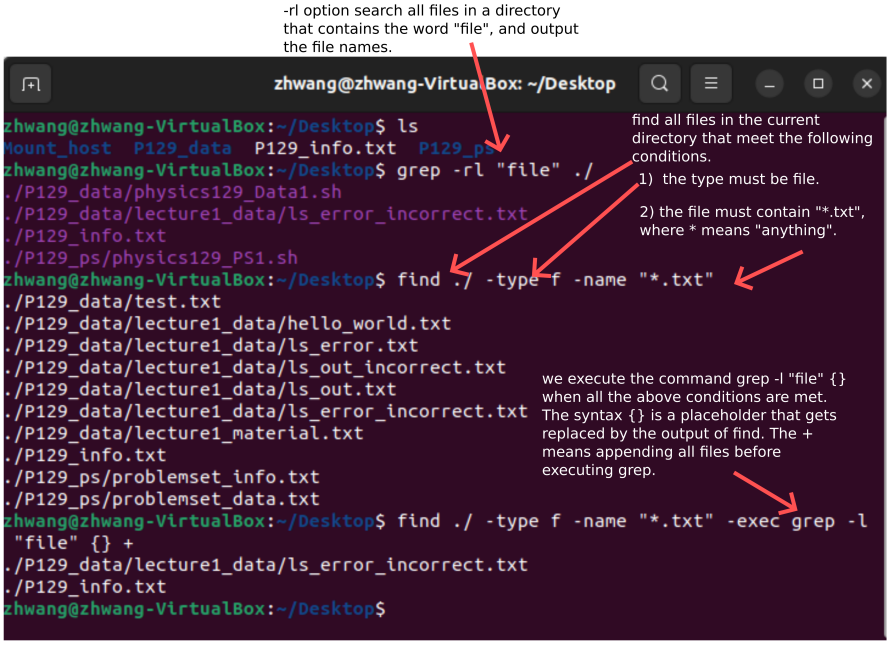


Figure 5: ”find” command.

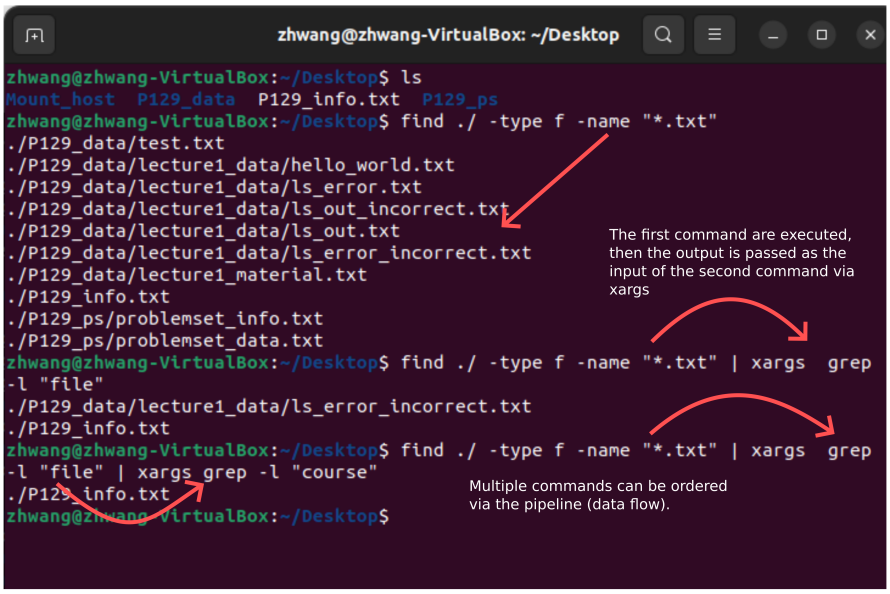


Figure 6: Pipelines.

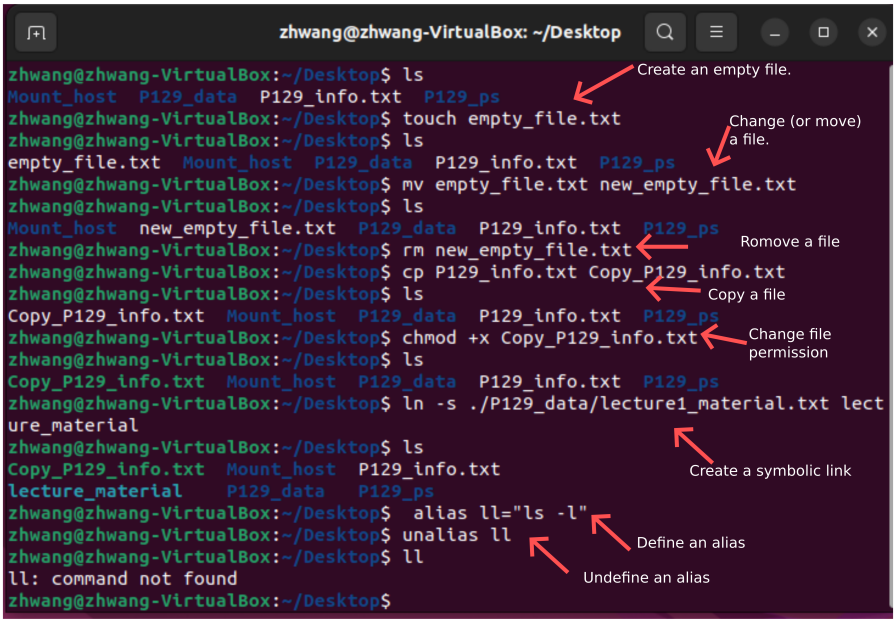


Figure 7: common Linux commands.

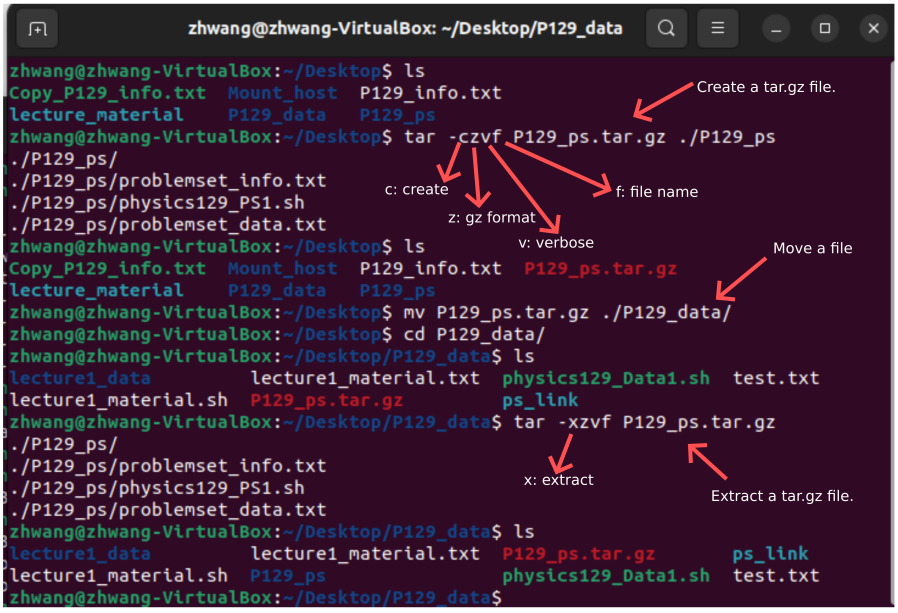


Figure 8: tar command.

2 bash script usages

A Bash script is a text file that contains a series of commands discussed above. It provides a great way to automate tasks and perform various operations in a Linux or Unix environment. We will explore the basic functionality of Bash scripting. A bash script usually has ".sh" file extension that can be executed. It has a shebang line that indicates the bash in the /bin directory will be used, #!/bin/bash. We usually find the hidden file in the use home directory, named ~/.bashrc, useful to customize bash shell based on our needs when we open the shell, e.g. alias or other script programs. We should note that it only applies to the local user, and if you want to apply system-wide changes, you should change /etc/bash.bashrc.

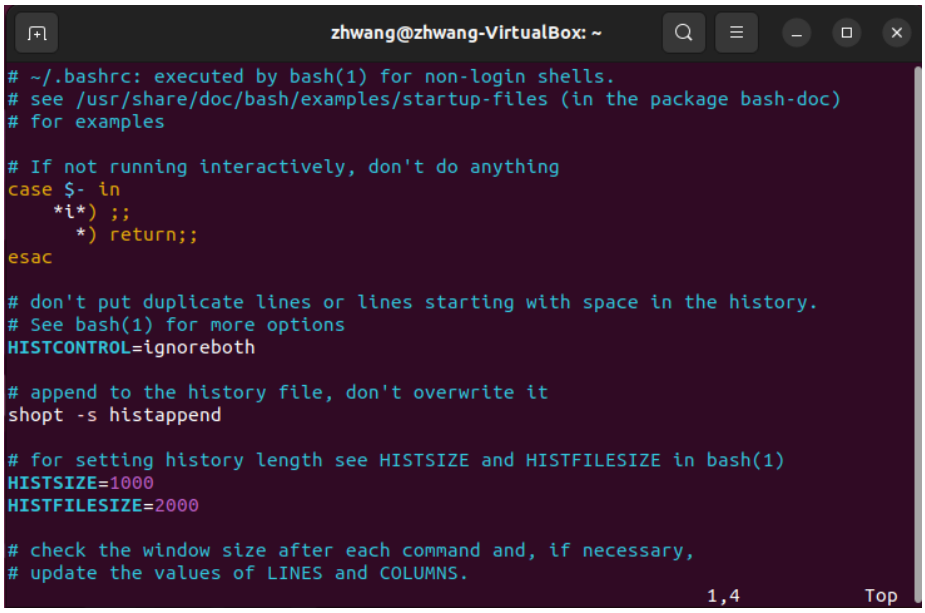


Figure 9: the .bashrc script

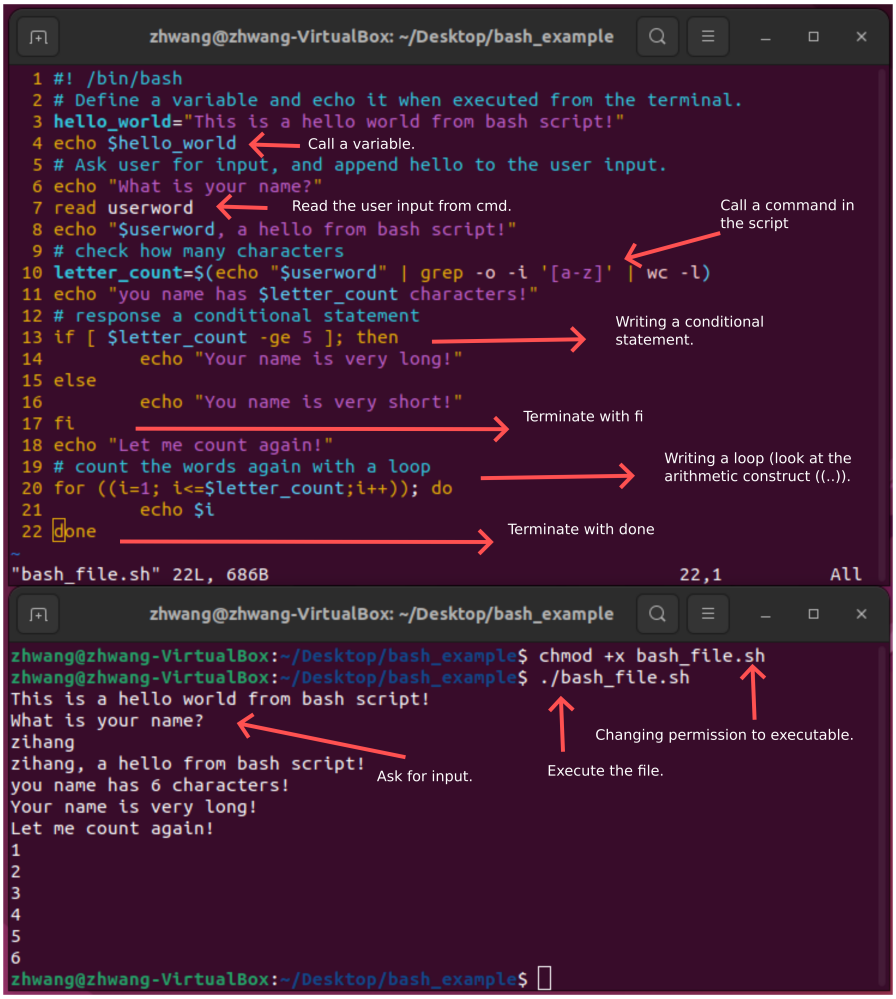


Figure 10: basics of bash scripts

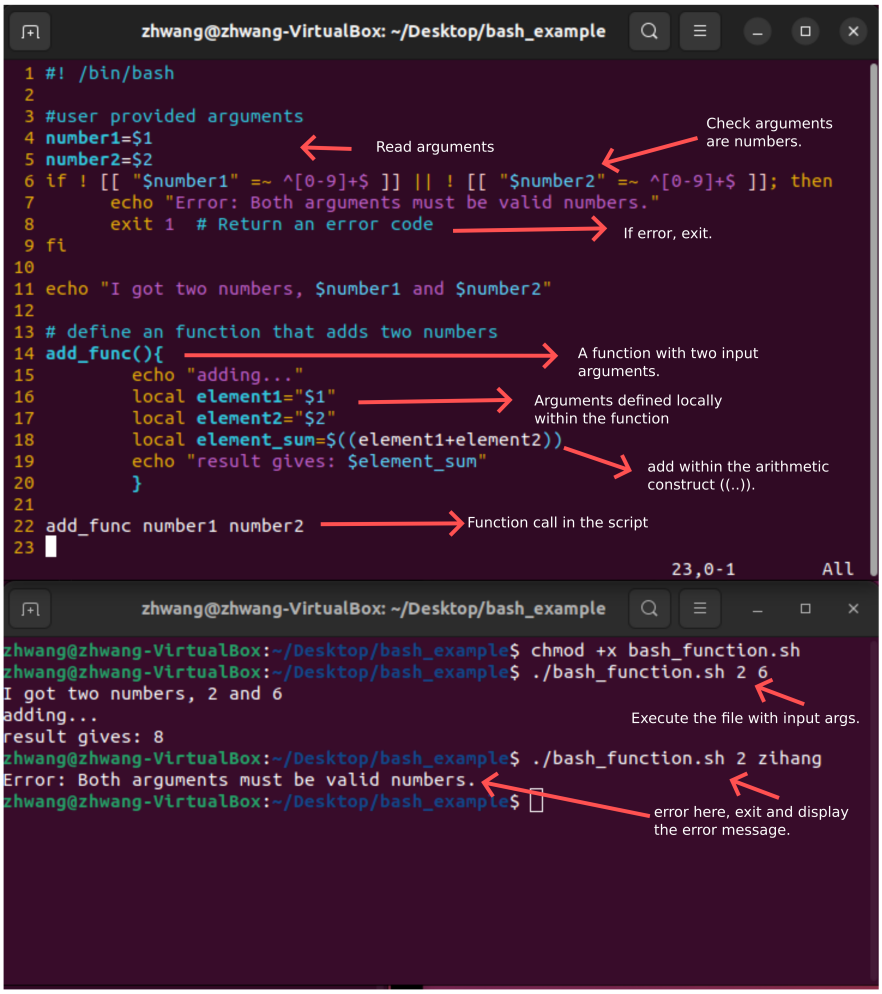


Figure 11: functions in bash scripts

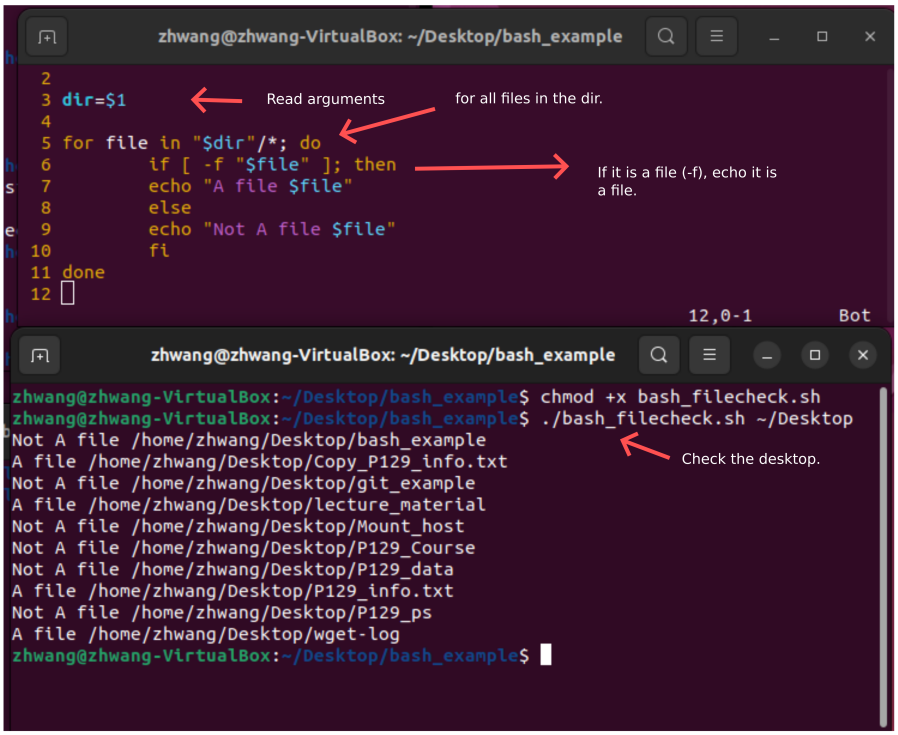
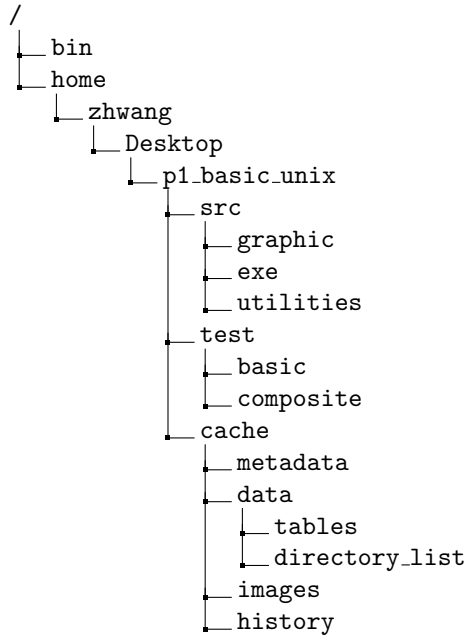


Figure 12: File management in bash

Problem 1: Basic UNIX File Management

In most projects, a directory tree is an essential tool for file management. Here, we will construct a directory tree and explore basic Linux commands. Below is an example of a complete directory tree, starting from the root "/".

Please submit **all** your commands (including errors) in a text file named "P1_cmd_history.txt" in the directory "/p1_basic_unix". For example, if you want to select the last 10 commands you entered and append them to a file, you can use the following 'history' command: "history | tail -n 10 >> P1_cmd_history.txt". Please note that by doing this, the last command in the text file is **guaranteed** to be the 'history' command above.



A

1. Construct the directory tree in the container. Hint: you do not need to start from the root, instead, starting with host, so you can directly access files from your local computer!

2. Move to "/p1_basic_unix", and add 3 **empty** ".txt" files: test_1.txt, test_2.txt, test_3.txt, to the directory "/p1_basic_unix/test/basic".

3. Stay in "/p1_basic_unix", and use the **echo** command to print your name and today's date to test_1.txt.

4. Stay in "/p1_basic_unix", use the **cat** command to print test_1.txt to the terminal.

5. Stay in "/p1_basic_unix", use the **ls -l** command to print test_1.txt to test_2.txt.

6. Stay in "/p1_basic_unix", make the test_1.txt file executable with **chmod +x**, and **append** the result of **ls -l** to test_2.txt.

B

1. Download the compressed tar file "P1_B.tar.gz" from the course website under Problem Sets, Downloads. Extract the tar file to the directory "/p1_basic_unix". Hint: use the "wget ..." command. **Please check the sha256sum!**

2. Stay in "/p1_basic_unix", move example.sh from "P1_B" to "/p1_basic_unix".

3. Stay in "/p1_basic_unix", rename two existing files in the directory "P1_B" from example_1.txt and example_2.txt to demo_1.txt and demo_2.txt.

4. Stay in "/p1_basic_unix", move those two newly named files to "/p1_basic_unix/src/exe" and "/p1_basic_unix/cache/data/tables".

5. Stay in "/p1_basic_unix", remove the directory "P1_B".

6. Stay in "/p1_basic_unix", create a symbolic link for the file demo_1.txt with the name demo_link.

7. Set an alias "ll" that defines the operation "ls -l".

C

1. Stay in "/p1_basic_unix", use **grep** to search for the keyword "statistics" in demo_1.txt, and using pipelines, print the result to a new file named "grep_stat_demo1.txt". Place the new file into the directory "/p1_basic_unix/src/utilities".

2. Stay in "/p1_basic_unix", perform a **grep** search for the keyword 'statistics' across all directories. Utilize pipelines to redirect the results into a new file named 'grep_stat_all.txt,' placing it within the directory "/p1_basic_unix/cache/images".

3. Stay in "/p1_basic_unix", use the **find** command to locate all files with a ".txt" extension and print them to the test_3.txt file.

4. Stay in "/p1_basic_unix", employ both the **find** and **grep** commands to search for the keyword 'statistics' within all files of the '.txt' format across all directories.

Submission to Github

For problem 1 submission, you are asked to create your own repository with git and push the ".tar.gz" file to the remote as an archive.

1. Using the **tar** command, compress the directory "/p1_basic_unix" into a **single** ".tar.gz" file named "p1_basic_unix.tar.gz".
2. Obtain the sha256sum by running "sha256sum p1_basic_unix.tar.gz".

Then, do the following for submitting your P1 to the remote.

1. Create a separate directory, /Archive_P1, and initialize git.
2. Copy your tar.gz file for the first problem to this repository.
3. Initialize the main branch, stage the change, and commit the change.
4. Following the discussion in the section, create your personal access token on github.
5. Commit to the remote repository. As what you did in the section, you need to first create the remote repository (with the same name) on github!

Problem 2: File Management and Bash Scripts

Bash scripts hold significant value in modern Linux system administration; they are used for automating tasks and performing various operations. In this problem, we will explore the fundamental uses of bash scripts.

In modern computing, file searching is critical for data extraction. The output data files from an instrument are typically labeled with information such as subject, year, month, date, and index (if there are multiple files). For example, in an electron scattering experiment, the instrument produces data files as binary files with names like:

$$\text{example\_file\_name}: \quad \text{electron\_scattering\_2023} - 10 - 04\text{\_sample\_index\_0.bin}$$

In this question, you are will manage the data files created by your collaborator who measure the energy lost in an inelastic electron scattering experiment.

1. Fork the problem /P_2 on GitHub, and then clone the forked repository. The directory tree has the following structure:

```
/
└── P2
    └── /Problem_1
        └── /electron scattering data
```

2. Imagine your collaborator accidentally output data files to the wrong directory, i.e. /Problem_1. There are 500 files of them, and you need to delete them. **write a **single** line on the terminal that does the job.**

3. Your future collaborators may need to address this issue again, but they may have no knowledge of Linux commands. Write a bash script that defines an alias named 'file_remove.' It should accept a single argument: the name of the target directory. Hint: Use your previous work.

4. Navigate to the directory /electron_scattering_data. Your collaborator has requested that you separate the files with odd indexes from those with even indexes and move them to two new directories within the current directory. The two directories should be named /electron_scattering_data/odd and /electron_scattering_data/even, respectively. Write a bash script to accomplish this task. Hint: Use a for loop.

5. Submit a **pull request** on github. we will later review your code and give you comments on your submission.

(optional) If you are interested and have time, decode the binary files above with **python** and infer the corresponding statistical distributions.

Problem 3: Number Conversions and Bash Scripts

Although less common, people use bash scripts to perform basic calculations or conversions. There are three types of numbers: decimal (base-10), binary (base-2), and hexadecimal (base-16). An example conversion is provided in Table 1. In this problem, you are asked to **write a bash script that converts**

Hexadecimal	Decimal	Binary
1	1	0001
2	2	0010
3	3	0011
4	4	0100
5	5	0101
6	6	0110
7	7	0111
8	8	1000
9	9	1001
A	10	1010
B	11	1011
C	12	1100
D	13	1101
E	14	1110
F	15	1111
10	16	00010000
1A	26	00011010
1F	31	00011111
20	32	00100000

Table 1: Examples on Hexadecimal, Decimal, and Binary Number Conversions

Division	Quotient	Remainder
125064 / 16	7816	8
7816 / 16	488	8
488 / 16	30	8
30 / 16	1	14
1 / 16	0	1

Table 2: Example: converting Decimal to hexadecimal via division remainders. In hexadecimal, it is 1E888.Or in binary, it is 11110100010001000.

a given decimal number to both hexadecimal and binary numbers. In addition, the program should only accept decimal values smaller than 100000. You are required to hard-code the conversions using information from both Table. 1 and Table. 2! Please copy your bash script into a directory named /Problem_3, and the outcome should be passed

to a .txt file with name “convertion_result.txt”, also in /Problem_3.

Push it to github with the repo name /Problem_3.

Problem 4: Version Control with Git.

Similar to what we have done in the section and write the answer in a README file under the repository you created in the section.

1. Checkout a different branch, called feature_branch. Create a readme file with “hello world!”. Then, stage, commit and push to the **feature_branch** and push to the remote.

2. After you push the feature_branch, merge the feature_branch with the main branch locally, and push to the remote. What do you see locally and remotely on github?

3. Modify the text in readme file from ”hello world!” to ”hello world from remote!” **on github manually**, and pull from the remote origin. Do you see the update?