

HW01

GitHub link: <https://github.com/yosunlu/repo759/tree/main/HW01>

task 1

I went through a) through c) and understand how to time code, how to submit my assignments with git, and what the recommended workflow is when it comes to working on my assignment.

task 2

- a. `cd somedir`
- b. `cat sometext.txt`
- c. `tail -n 5 sometext.txt`
- d. `tail -n 5 *.txt`
- e. `for ((i = 0; i <= 6; i++)); do echo "$i"; done`

task 3

- a. `no`
- b. `14.1.1`
- c. `gromacs/cuda-12.2-mpich/2023.3`
 - `nvidia/cuda/10.2.2`
 - `nvidia/cuda/11.3.1`
 - `nvidia/cuda/11.8.0`
 - `nvidia/cuda/12.1.0`
 - `nvidia/cuda/12.5.0`
 - `nvidia/nvhpc-hpcx-cuda12/23.11`

gromacs/cuda-12.2/2023.3

nvidia/cuda/11.0.3

nvidia/cuda/11.6.0

nvidia/cuda/12.0.0

nvidia/cuda/12.2.0

nvidia/nvhpc-hpcx-cuda11/24.5

nvidia/nvhpc-hpcx-cuda12/24.5

- d. anaconda/mini/4.9.2 is a lightweight version of the Anaconda distribution that provides essential tools for managing Python environments and packages, useful for data science and machine learning workflows.

task 5

- a. Where the sbatch command was executed.
- b. **Slurm Job ID** is a unique identifier assigned to each job when it is submitted to the Slurm workload manager. This Job ID is used to track and manage the job throughout its lifecycle, from submission to execution and completion.
- c. `squeue -u $USER`
- d. `scancel $SLURM_JOB_ID`
- e. `#SBATCH --gres=gpu:1` specifies that the job requires 1 GPU
- f. `#SBATCH --array=0-9` specifies that the Slurm job is part of a **job array** consisting of **10 jobs**, with array indices ranging from 0 to 9