Summary of Instructions

1.) Copy “ch447_547/Unbiased_Simulation_Only_Codes/” to “ch447_547/username/”

2.) Move into your new “ch447_547/username/Unbiased_Simulation_Only_Codes/”

3.) Copy your pdb file of the lysozyme into the “base_lysozyme” folder.

4.) Create a “{}_config.sh” file which will contain information about your system. I typically name this config.sh file with descriptions for the specific conditions that I am running.
General Example: “{salt_concentration}_{protein_name}_{planned_run_time}_config.sh
Specific Example: “Na_100_Mg_6_lyzosyme_new_forcefields_100ns_config.sh”

In the config.sh file we will include the following text.

```
# config.sh

## protein related
pdb="lysozyme_1lyd.pdb"
protname="lysozyme"

## directory related
config_dir="config"
em_dir="em"
ion_dir="ions"
nvt_dir="nvt"
npt_dir="npt"
prod_dir="pro"

## salt related
na_conc=0.1
mg_conc=0.006

## run name
#run_name="Na_100_Mg_6_lysozyme_new_forcefields_100ns"
```

5.) Run the script “1_scratch_md_generalized_positive_system.sh” by typing
“sbatch 1_scratch_md_generalized_positive_system.sh {base_dir} {run_name}”

6.) Make sure to check that no errors are given in output and that system is neutral by going into {run_name}/config/tleap.log.

7.) Run the script “2_run_em_generalized.sh” by typing in command
“sbatch 2_run_em_generalized.sh {run_name}”

8.) Make sure to check that energy has converged before going on to next step.

9.) Check if temperature has stabilized and pressure has stabilized around 0 bar at end of npt simulation.

10.) Run the following python command.

“python3 1_write_GROMACS_production_codes_generalized.py -run_name {run_name} -prot_name {prot_name} ”