1 Prepare folders for upload

In my opinion, the best practice is to upload all the necessary files for getting the simulation started and all the files that were created during the simuation. Therefore, the upload consists of the following files: "*.xtc", "*.edr", "*.tpr", "*.top", "*.mdp", "*.ndx", "*.gro", "*.cpt", "*.log". The index file here is the one that you used for calling the "gmx grompp ...". I also include a comressed folder with all the topology files as they are called by the "*.top" file. So the goal now is to create the folders.

1. Choose a path into where you create all the folders
2. Create one folder per one system
    - Copy/move in files used for the "gmx grompp" command: "*.top", "*.mdp", "*.ndx", "*.gro"
    - Copy/move in the "*.tpr" used for generating the trajectory
    - Copy/move in the resulting files: "*.xtc", "*.edr", "*.log", "*.cpt"
    - Copy/move in the folder with topology files and compress it
3. Prepare all the systems you want to upload in the same way. Make sure all the folders are at the same path

2 Create README.yaml files

This part creates the README.yaml, but it also creates the two extra trajectories: one with reduced saving frequency and another one without water molecules (only when water is recognised, to be updated). The original trajectory file is moved out of the folder to "../original_trajectories/" (not yet). This has to be done, since later the whole content of the folders will be uploaded to ZENODO. In this part, you can also choose to provide an information of equlibration time of your simulation (not yet).

1. Update path at the very bottom of "ManageSimulations.py"
2. Run "ManageSimulations.py"

3 How to upload to ZENODO

Files can be uploaded to ZENODO with the help of a script. The script requires a security token. Unfortunately, I have not succeeded to create new repositories in ZENODO with the help of a script, so this part has to be done manually.

1. Create a ZENODO token
    - go to `https://zenodo.org/account/settings/applications/`, create a token, and copy it
    - write the token to the ”zenodo_upload.sh” script. This is the only part that has to be modified in this script.
2. Create repositories in ZENODO
    - go to `https://zenodo.org/deposit/new` and create a new repository
    - Fill all the info with astrerixes, so that you can then save the repository
    - Also choose to ”reserve DOI” under the ” Digital Object Identifier ”
    - After you reserved the DOI, the adress in browser changes, copy it
    - Paste the adress containing DOI into a dictonary in the ”UploadToZENODO.py” script
3. Create a dictonary in the ”UploadToZENODO.py” script
    - This dictonary connects DOIs with systems.
    - The keys in the dictonary are names of the folders with your systems that you prepared before
    - The values in the dictonary are the adresses containing DOI that you copied from ZENODO
4. Change the path in ”UploadToZENODO.py”, so it points to the place with your folders.
5. You are ready to run the ”UploadToZENODO.py” script!
    - This script tracks the progress of uploads and repeats an upload until the whole file is successfully in ZENODO.