MD simulation with HPC (protein-protein interaction)

1. Use the DROIDS GUI to prep the files for MD simulation:
   1. Bound: 6m17\_bound
   2. Unbound: 6m17\_unbound

Graphical user interface, application

Description automatically generated

1. Press the following buttons and get thru the initial set up
   1. Dry and reduce structure (run pdb4amber)
   2. Make MD, cpptraj, and DROIDS control files (.ctl)
   3. Create sequence and structural alignment (UCSF chimera)
   4. Generate topology and coordinate files (teleap)
2. When you get the “launch MD run-make take hours” button, click on it. This will create the .prmtop and other files. And also the random spacer files. As soon as you see the minimization run starting close all the file and runs. ,
3. Now transfer the DROIDS folder over to your folder in HPC.
4. After you transfer it over, make sure to add the following files to the droids folder
   1. driver.sh
   2. min\_heat.sh
   3. eq.sh
   4. rand\_prod.sh
   5. info\_flux.sh
5. All you have to do is change the input in driver.sh files to start the run
   1. Line 2 input\_1=”6m17\_bound”
   2. Line 3 input\_2=”6m17\_unbound”
   3. Line 4 num\_runs=100
6. Navigate into the droids folder and start the run using the following command
   1. bash driver.sh
7. When the runs are done, move the generated .nc files over to another folder
8. Now transfer the droids folder over back to your linux machine
9. Now continue with other analyses by pressing the following button
   1. “parse / prepare files for DROIDS”

MAJOR NOTES

1. You have access to a shared folder on the HPC. It has 70TB of space. Use it to run the simulations
   1. Path is /shared/rc/silico
   2. Only you and me have access to silico
2. Here are the description of the five bash files
   1. driver.sh – Main driver bash file for the MD simulations.
   2. min\_heat.sh – Slurm script file to start the minimization and heating run.
      1. Gets the input and direction from driver.sh
      2. change –mail-user and –account
   3. eq.sh – Slurm script file to start the equilibration run.
      1. This script only executes if the min\_heat.sh script finishes successful.
      2. Gets the input and directions from driver.sh
      3. Change –mail-user and –account
   4. rand\_prod.sh -Slurm script file to start the rand and production runs. T
      1. This script only executes if the eq.sh completes successfully
      2. Gets the input and directions from the driver.sh
      3. Each random run is followed by its respective production run
      4. 100 random-production run pairs are started simultaneous based on the availability of a100 and v100 gpus on the cluster
         1. –array command in the driver.sh in line 9 and line 13 says the HPC to start at most 100 rand/production runs at a time
      5. change –mail-user and –account
   5. info\_flux.sh – Slurm script file to generate the atom info and fluctuation files.
      1. This script files only executes if the 100 rand\_prod runs are successfully completed.
      2. Gets the input and directions from driver.sh
      3. change –mail-user and –account
      4. This also runs 100 analyses at the same time based on the number of computers available