GROMACS patched to PLUMED on Euler 01/09/2024

1. Switch to new software stack: $ env2lmod
2. $ module load gcc/9.3.0
3. $ module load cmake/3.26.3
4. $ module load python/3.7.4
5. (you are in your home directory on Euler) $ mkdir programs
6. $ cd programs
7. Now get plumed from github:
   git clone https://github.com/plumed/plumed2.git
8. $ cd plumed2
9. $ ./configure --prefix=/cluster/home/hansenni/programs/plumed2_INSTALL
10. $ make -j4
11. $ make install
12. $ source sourceme.sh
13. Now download Gromacs 2023.2 from https://manual.gromacs.org/2023.2/download.html
    Move the tar ball into the programs directory, change into the programs directory and unpack it there.
14. $ cd gromacs-2023.2
15. $ plumed patch -p
    the best matching code/version in our case is gromacs-2023.2
16. $ mkdir build
17. $ cd build
18. $ cmake .. -DGMX_BUILD_OWN_FFTW=ON -DCMAKE_INSTALL_PREFIX=/cluster/home/hansenni/programs/gromacs-2023.2_plumed2_INSTALL
19. $ make -j4
20. $ make install
21. $ source /cluster/home/hansenni/programs/gromacs-2023.2_plumed2_INSTALL/bin/GMXRC.bash
22. Now you are ready to start for using GROMACS in conjunction with PLUMED. If you type
    $ gmx mdrun -h
    in the terminal the option -plumed should be listed under the available options.
23. Enter the lines:
    source /cluster/home/hansenni/programs/plumed2/sourceme.sh
    source /cluster/home/hansenni/programs/gromacs-2023.2_plumed2_INSTALL/bin/GMXRC.bash
    at the end of your .bashrc
24. Now obtain the umbrella integration program from github:
    $ pip install --user git+https://github.com/M-R-Schaefer/umbrella_integration
25. Get exercise files from github:
    git clone https://github.com/hansenniels/freeenergy_tutorial.git
26. The umbrella sampling simulation in water can now be started with
    sbatch < start_sim_euler_slurm.sh

Analyze US simulations on Euler 01/09/2024

1. Switch to new software stack: $ env2lmod
2. **WHAM** (we use an older (pre-installed) version of GROMACS which can still read pdo-files):

   ```
   $ module load python/3.7.4
   $ module load gcc/8.2.0
   $ module load openmpi/4.0.2
   $ module load gromacs/2021.2
   $ python prepare_gmx_wham.py
   $ gmx_mpi wham -ip pdo-files.dat -o pmf_WHAM.xvg -min 0.39 -max 1.15
   ```

   to display the PMF use xmgrace

   ```
   $ module load xmgrace
   ```

3. **UI**:

   ```
   $ module load gcc/11.4.0
   $ module load python/3.11.6
   $ python prepare_UI.py
   $ ./command_UI_python
   ```

   The package will be installed in a local repository at $HOME/.local. Since this is the default path for user-installed python packages, there should be no need to adjust PYTHONPATH.

4. **MBAR**: requires the package pymbar version 4 which comes with the alchemlyb package. For installing the required packages on Euler locally perform the following steps:

   ```
   $ pip install --user alchemlyb
   $ python umbrella_sampling_MBAR.py
   ```

   The package will be installed in a local repository at $HOME/.local. Since this is the default path for user-installed python packages, there is no need to adjust PYTHONPATH.