GROMACS patched to PLUMED on Euler 01/07/2023

1. Switch to new software stack: $ env2lmod
2. $ module load gcc/9.3.0
3. $ module load cmake/3.25.0
4. (you are in your home directory on Euler) $ mkdir Programs
5. $ cd Programs
6. Download Plumed (2.7.1) from https://github.com/plumed/plumed2/releases/tag/v2.7.1 and copy it to the Programs folder in Euler.
7. Unpack the tar ball:
   gunzip plumed-2.7.1.tgz
   tar -xvf plumed-2.7.1.tar
8. $ cd plumed-2.7.1
9. $ ./configure --prefix=/cluster/home/hansenni/Programs/plumed-2.7.1_INSTALL
10. $ make -j4
11. $ make install
12. $ source sourceme.sh
13. Now download Gromacs 2021.2 from
    https://manual.gromacs.org/documentation/2021.2/download.html
    Move the tar ball into the Programs directory, change into the Programs directory and unpack it there.
14. $ cd gromacs-2021.2
15. $ plumed patch -p
    the best matching code/version in our case is gromacs-2021
16. $ mkdir build
17. $ cd build
18. $ cmake .. -DGMX_BUILD_OWN_FFTW=ON -DCMAKE_INSTALL_PREFIX=/cluster/home/hansenni/Programs/gromacs-2021.2_plumed-2.7.1_INSTALL
19. $ make -j4
20. $ make install
21. $ source /cluster/home/hansenni/Programs/gromacs-2021.2_plumed-2.7.1_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/plumed-2.7.1/sourceme.sh
    source /cluster/home/hansenni/Programs/gromacs-2021.2_plumed-2.7.1_INSTALL/bin/GMXRC.bash
    at the end of your .bashrc
24. Now the exercise files can be downloaded as will be explained in the course.

Analyze US simulations on Euler 01/10/2023

1. Switch to new software stack: $ env2lmod
2. **WHAM**: $ module load python/3.7.4
   $ python prepare_gmx_wham.py
   $ gmx wham -ip pdo-files.dat -o pmf_WHAM.xvg -min 0.39 -max 1.15

   In my case the last command resulted in a segmentation fault for unknown reasons. Therefore, I used the preinstalled GROMACS for this task:

   $ module load gcc/8.2.0
   $ module load openmpi/4.0.2
   $ module load gromacs/2021.2
   $ 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**: Umbrella integration requires python2. First clone the code from the Programs directory:
   $ git clone https://github.com/ATB-UQ/umbrella_integration.git
   Then load python 2.7.14 and issue the UI call
   $ module load python/2.7.14
   $ python ~/Programs/umbrella_integration/xxx (*see command file*)
   The error message about the plot can be ignored (missing matplotlib) since the PFM is also written to file (pmf_UI.dat) and can be plotted separately. However, you can install matplotlib locally using

   $ pip install --user matplotlib

   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.

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:

   $ env2lmod
   $ module load gcc/6.3.0
   $ module load gcc/8.2.0
   $ module load python/3.8.5
   $ 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.