INSTALLATION AND PATCHINGOF PLUMED WITH AMBER AND GROMACS

PLUMED INSTALLATION ::

Download PLUMED using one of the following methods :

git clone https://github.com/plumed/plumed2.git

https://drive.google.com/file/d/1So2SnPxu5_yn7K8T4WuQjKMmAOBcChe5/view

Once downloaded go to the PLUMED home folder $PLUMED_HOME and configure it by running following command !

#! [./configure --enable-shared]
NOW RUN [make -j8]
#! RUN [source $PLUMED_HOME/sourceme.sh]

once it done check your plumed executable path.

AMBER INSTALLATION AND PATCHING WITH PLUMED ::

Download Ambertools using website of AMBER :: http://ambermd.org/GetAmber.php#ambertools

Once downloaded follow the instruction to install the amber :-

untar Ambertools "tar -xvf AmberTools.tar.bz2"**

go to Amber home folder and type export AMBERHOME=`pwd`

Now configure with gnu or intel compiler ./configure gnu/intel

To enable MPI ./configure -mpi gnu/intel

after configuration open config.sh file and give the Plumed sghared library path to Patch AMBER with PLUMED

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# PLUMED related variables:
PLUMED_INCLUDE_FILE=$PLUMED_HOME/src/lib/Plumed.inc
PLUMED_LOAD=Plumed.o -ldl -Wl,-export-dynamic
PLUMED_DEPENDENCIES=Plumed.o
```

Now , type make -j16 to compile the amber which is now patche with plumed.

GROMACS INSTALLATION AND PATCHING WITH PLUMED ::

Download GROMACS from the website or by typing :

wget ftp://ftp.gromacs.org/pub/gromacs/gromacs-2016.tar.gz

untar the gromacs then go to the GMX_HOME and type :

plumed-patch --shared -p -e gromacs-2016 (or any version which is compatible with plumed)

{THIS WILL LINK LIBRARIES OF PLUMED WITH GROMACS TO PATCH}

now make a build directory and go to that directory then type :

cmake .. -DGMX_BUILD_OWN_FFTW=ON -DGMX_MPI=ON

[you may need latest version of cmake and fftw to be download if not then go onn type make -j16 if it gives you error then follow the following steps]

DOWNLOAD fftw BY RUNNING THIS IN TERMINAL [wget http://www.fftw.org/fftw-3.3.8.tar.gz]

"if above not works then download and copy and "EXTRACT IT USING [tar -xvf fftw-3.3.8.tar.gz]

GO TO $GROMACS_HOME/build/src/contrib/fftw AND THEN RENAME FFTW

cp fftw-3.3.8.tar.gz fftw.tar.gz !

COMMENT OR REPLACE THE FOLLOWING FILE.... !

vi $GROMACS_HOME/build/src/contrib/fftw/fftwBuild-prefix/src/fftwBuild-stamp/verify-fftwBuild.cmake

NOW RUN 'make -j8' IN $GROMACS_HOME/build/src/contrib/fftw FOLDER

ONCE IT DONE GO BACK TO THE build DIRECTORY AND RUN THE 'make -j16'

Now check weather the plumed is patched with gromacs by typing :

gmx_mpi mdrun -h | grep plumed

```
  gmx_mpi mdrun -h

         [-multidir [<dir> [...]]] [-plumed [<.dat>]] [-membed [<.dat>]]
 -plumed [<.dat>]           (plumed.dat)     (Opt.)

GROMACS reminds you: "Restraint! What possible restraint?" (Joseph Conrad)
```

!!THANKS!!