https://manual.gromacs.org/documentation/#latest-releases

<https://ftp.gromacs.org/gromacs/gromacs-2022.4.tar.gz>

<https://ftp.gromacs.org/regressiontests/regressiontests-2022.4.tar.gz>

tar xfz gromacs-2022.4.tar.gz

cd gromacs-2022.4000.

00..00000000000000000

…..

mkdir build

cd build

apt install cmake

apt-get install fftw-dev

cmake .. -DGMX\_BUILD\_OWN\_FFTW=ON -DREGRESSIONTEST\_DOWNLOAD=ON -DGMX\_GPU=CUDA -DCUDA\_TOOLKIT\_ROOT\_DIR=/apps/compiler/cuda-12.0 -DGMX\_MPI=OFF -DCMAKE\_CXX\_COMPILER=g++ -DCMAKE\_C\_COMPILER=gcc -DCMAKE\_INSTALL\_PREFIX=/apps/compiler/gromacs-2022.4

cmake .. -DGMX\_BUILD\_OWN\_FFTW=ON -DREGRESSIONTEST\_DOWNLOAD=OFF

cmake .. -DGMX\_BUILD\_OWN\_FFTW=OFF -DREGRESSIONTEST\_DOWNLOAD=OFF -DGMX\_GPU=CUDA -DCUDA\_TOOLKIT\_ROOT\_DIR=/usr/local/cuda-12.0 -DGMX\_MPI=ON -DREGRESSIONTEST\_PATH=/opt/regressiontests-2022

#cmake .. -DGMX\_GPU=CUDA -DGMX\_MPI=ON -DCMAKE\_INSTALL\_PREFIX=/apps/compiler/gromacs-2022.2

cmake -B /apps/Compile/gromes-2022 -DGMX\_BUILD\_OWN\_FFTW=ON -DREGRESSIONTEST\_DOWNLOAD=ON

go to cd /apps/Compile/gromes-2022 && make -j32 && make -j32 install

note= where the make file is create run make that file

make -j32

make -j32 check

sudo make install

source /usr/local/gromacs/bin/GMXRC

(base) root@linux:/opt/gromacs-2022.4# gmx –version ##Gromecs checked

:-) GROMACS - gmx, 2022.4 (-:

Executable: /usr/local/gromacs/bin/gmx

Data prefix: /usr/local/gromacs

Working dir: /opt/gromacs-2022.4

Command line:

gmx --version

GROMACS version: 2022.4

Precision: mixed

Memory model: 64 bit

MPI library: thread\_mpi

OpenMP support: enabled (GMX\_OPENMP\_MAX\_THREADS = 128)

GPU support: disabled

SIMD instructions: AVX2\_256

CPU FFT library: fftw-3.3.8-sse2-avx-avx2-avx2\_128

GPU FFT library: none

RDTSCP usage: enabled

TNG support: enabled

Hwloc support: disabled

Tracing support: disabled

C compiler: /usr/bin/cc GNU 9.4.0

C compiler flags: -mavx2 -mfma -pthread -Wno-missing-field-initializers -fexcess-precision=fast -funroll-all-loops -O3 -DNDEBUG

C++ compiler: /usr/bin/c++ GNU 9.4.0

C++ compiler flags: -mavx2 -mfma -pthread -Wno-missing-field-initializers -fexcess-precision=fast -funroll-all-loops -fopenmp -O3 -DNDEBUG

1. MPI support >> -DGMX\_MPI=on
2. GPU-aware MPI support >> GMX\_MPI=ON
3. cmake –version
4. Fast Fourier Transform library>>>

cmake-DGMX\_FFT\_LIBRARY=<name> {<name> ="fftw3", "mkl", or

"fftpack" }

1. Using FFTW

cmake-DGMX\_BUILD\_OWN\_FFTW=ON

1. Using MKL

-DGMX\_FFT\_LIBRARY=mkl

7) If you need to customize this further, use

cmake -DGMX\_FFT\_LIBRARY=mkl \

-DMKL\_LIBRARIES="/full/path/to/libone.so;/full/path/to/libtwo.so" \

-DMKL\_INCLUDE\_DIR="/full/path/to/mkl/include"

8) Using ARM Performance Libraries

cmake -DGMX\_FFT\_LIBRARY=fftw3 \

-DFFTWF\_LIBRARY="${ARMPL\_DIR}/lib/libarmpl\_lp64.so" \

-DFFTWF\_INCLUDE\_DIR=${ARMPL\_DIR}/include

9) CUDA GPU acceleration

you have the CUDA Toolkit installed, you can use "cmake" with:

cmake .. -DGMX\_GPU=CUDA -DCUDA\_TOOLKIT\_ROOT\_DIR=/usr/local/cuda

NOTE- go to /opt/gromacs-2022.4/build

#cd /opt/gromacs-2022.4/build

# cmake .. -DGMX\_GPU=CUDA -DCUDA\_TOOLKIT\_ROOT\_DIR=/usr/local/cuda-12.0

# gmx --version

###Error in user input:

'–version' is not a GROMACS command.

#make

#make check

#make install

cat /etc/profile.d/gromacs-2022.sh

export PATH=/usr/local/gromacs/bin:${PATH}

export LD\_LIBRARY\_PATH=/usr/local/gromacs/lib:${LD\_LIBRARY\_PATH}

export C\_INCLUDE\_PATH=/usr/local/gromacs/include:${C\_INCLUDE\_PATH}