Gromacs 4.5.5

Webpage

http://www.gromacs.org/

Version

4.5.5

Tools for Compiling

- Intel Composer XE 2011 sp1.8.273
- Intel MPI 4.0.2.003

Necessary Files for Compiling

- gromacs-4.5.5.tar.gz

Procedure of Compiling

CPU Edition

```
#!/bin/csh -f
umask 022
set file_gromacs=/home/users/${USER}/build/gromacs455/gromacs-4.5.5.tar.gz
set work=/save/users/${USER}
# mpicc -> mpiicc
set path=(/home/users/${USER}/compiler/ccpg/intel-12.0 $path)
#-------------------------------------------------------------------------------
cd ${work}
rm -rf ${work}/gromacs455
if (-d gromacs-4.5.5) then
  mv gromacs-4.5.5 gromacs-4.5.5-erase
  rm -rf gromacs-4.5.5-erase &
endif
tar xzf ${file_gromacs}
cd gromacs-4.5.5
./configure --enable-double --disable-la-files --enable-mpi --with-fft=mkl --with-external-blas --with-external-lapack --with-gsl --
prefix=/local/apl/pg/gromacs455
make -j12 ASFLAGS="-O3 -xHost" CCASFLAGS="-O3 -xHost" CFLAGS="-O3 -xHost"
mkdir ${work}/gromacs455
make install
```

GPU Edition

```
#!/bin/csh -f
umask 022
set file_gromacs=/home/users/${USER}/build/gromacs455/gromacs-4.5.5.tar.gz
set work=/save/users/${USER}
#-------------------------------------------------------------------------------
cd ${work}
if (-d gromacs-4.5.5) then
  mv gromacs-4.5.5 gromacs-4.5.5-erase-gpu
  rm -rf gromacs-4.5.5-erase-gpu &
endif
tar xzf ${file_gromacs}
cd gromacs-4.5.5
setenv OPENMM_ROOT_DIR /local/apl/pg/openmm41
cmake . -DGMX_OPENMM=ON -DCMAKE_INSTALL_PREFIX=/local/apl/pg/gromacs455
make mdrun
make install-mdrun
```