

Gromacs 2016.3 for Primargy

Webpage

<http://www.gromacs.org/>

Version

2016.3

Tools for Compiling

- Intel Compiler 16.0.2
- Intel MPI 5.1.3.181
- cmake 2.8.12
- g++ (GCC) 4.9.2

Necessary Files for Compiling

- gromacs-2016.3.tar.gz

Procedure of Compiling

```
#!/bin/csh -f
umask 022
set file_gromacs=/home/users/${USER}/build/gromacs2016.3/gromacs-2016.3.tar.gz
set prefix=/local/apl/pg/gromacs2016.3
set work=/work/users/${USER}
#-----
cat <<EOF | scl enable devtoolset-3 csh
umask 022
cd ${work}
if (-d gromacs-2016.3) then
  mv gromacs-2016.3 gromacs-erase
  rm -rf gromacs-erase &
endif
tar xzf ${file_gromacs}
cd gromacs-2016.3
#
setenv CC icc
setenv CXX icpc
setenv F77 ifort
setenv F90 ifort
setenv FC ifort
mkdir rccs-s
cd rccs-s
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=OFF \
  -DGMX_THREAD_MPI=OFF \
  -DGMX_FFT_LIBRARY=mkl \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
mkdir rccs-d
cd rccs-d
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=OFF \
```

```

-DGMX_DOUBLE=ON \
-DGMX_THREAD_MPI=OFF \
-DGMX_FFT_LIBRARY=mkl \
-DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
setenv CC mpiicc
setenv CXX mpiicpc
setenv F77 mpiifort
setenv F90 mpiifort
setenv FC mpiifort
mkdir rccs-mpi
cd rccs-mpi
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix} \
-DMAKE_VERBOSE_MAKEFILE=ON \
-DGMX_MPI=ON \
-DGMX_GPU=OFF \
-DGMX_DOUBLE=OFF \
-DGMX_THREAD_MPI=OFF \
-DGMX_FFT_LIBRARY=mkl \
-DMPIEXEC=/opt/intel/impi/5.1.3.181/intel64/bin/mpirun \
-DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
mkdir rccs-mpi-d
cd rccs-mpi-d
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix} \
-DMAKE_VERBOSE_MAKEFILE=ON \
-DGMX_MPI=ON \
-DGMX_GPU=OFF \
-DGMX_DOUBLE=ON \
-DGMX_THREAD_MPI=OFF \
-DGMX_FFT_LIBRARY=mkl \
-DMPIEXEC=/opt/intel/impi/5.1.3.181/intel64/bin/mpirun \
-DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
EOF
```