Gromacs 4.6.1

Webpage

http://www.gromacs.org/

Version

4.6.1

Tools for Compiling

- gcc version 4.4.6
- Cuda compilation tools, release 5.0, V0.2.1221
- Intel MPI 4.0.2.003

Necessary Files for Compiling

- gromacs-4.6.1.tar.gz
- fftw-3.3.2.tar.gz

Procedure of Compiling

```
#!/bin/csh -f
umask 022
set file_gromacs=/home/users/${USER}/build/gromacs461/gromacs-4.6.1.tar.gz
set file_fftw3=/home/users/${USER}/build/gromacs461/fftw-3.3.2.tar.gz
set work=/work/users/${USER}
set prefix=/local/apl/pg/gromacs461
#------------------------------------------------------------------------------
cd ${work}
if (-d gromacs-4.6.1) then
  mv gromacs-4.6.1 gromacs-4.6.1-erase
  rm -rf gromacs-4.6.1-erase &
endif
tar xzf ${file_gromacs}
cd gromacs-4.6.1
mkdir -p src/contrib/fftw/gmxfftw-prefix/src
cp ${file_fftw3} src/contrib/fftw/gmxfftw-prefix/src
#
cmake28 . -DCMAKE_INSTALL_PREFIX=${prefix} \
    -DGMX_MPI=OFF \
    -DGMX_GPU=ON \
    -DGMX_DOUBLE=OFF \
    -DGMX_BUILD_OWN_FFTW=ON \
    -DREGRESSIONTEST_DOWNLOAD=OFF
make
make install
make clean
#
cmake28 . -DCMAKE_INSTALL_PREFIX=${prefix} \
    -DGMX_MPI=ON \
    -DGMX_GPU=OFF \
    -DGMX_DOUBLE=OFF \
    -DGMX_BUILD_OWN_FFTW=ON \
    -DMPIEXEC=/opt/intel/impi/4.0.2.003/intel64/bin/mpirun \
    -DREGRESSIONTEST_DOWNLOAD=OFF
make
make install
make clean
#
cmake28 . -DCMAKE_INSTALL_PREFIX=${prefix} \
    -DGMX_MPI=OFF \
    -DGMX_GPU=OFF \
    -DGMX_DOUBLE=ON \
    -DGMX_BUILD_OWN_FFTW=ON \
    -DREGRESSIONTEST_DOWNLOAD=OFF
make
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cmake28 . -DCMAKE_INSTALL_PREFIX=${prefix} \
    -DGMX_MPI=ON \
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    -DMPIEXEC=/opt/intel/impi/4.0.2.003/intel64/bin/mpirun \
    -DREGRESSIONTEST_DOWNLOAD=OFF
make
make install
make clean
```
