

Gromacs 4.6.5 for Primargy RX300/CX250

Webpage

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

Version

4.6.5

Tools for Compiling

- Intel Compiler 13.1.1
- Cuda compilation tools, release 5.0, V0.2.1221
- Intel MPI 4.1.3.049
- cmake 2.8

Necessary Files for Compiling

- gromacs-4.6.5.tar.gz

Attention

Setting `GMX_CPU_ACCELERATION=AVX_256` makes two fails in freeenergy of regressiontests.

Procedure of Compiling

```
#!/bin/csh -f
umask 022
set file_gromacs=/home/users/${USER}/build/gromacs465/gromacs-4.6.5.tar.gz
set work=/work/users/${USER}
set prefix=/local/apl/pg/gromacs465
set sse41_prefix=/local/apl/pg/gromacs465_sse41
#-----
cd ${work}
if (-d gromacs-4.6.5) then
  mv gromacs-4.6.5 gromacs-4.6.5-erase
  rm -rf gromacs-4.6.5-erase &
endif
tar xzf ${file_gromacs}
cd gromacs-4.6.5
#
setenv CC icc
setenv CXX icpc
setenv F77 ifort
setenv F90 ifort
setenv FC ifort
mkdir rccs-gpu
cd rccs-gpu
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=ON \
  -DGMX_DOUBLE=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_MPI=OFF \
-DGMX_GPU=OFF \
-DGMX_DOUBLE=ON \
-DGMX_FFT_LIBRARY=mkl \
-DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
mkdir rccs-d-sse41
cd rccs-d-sse41
cmake28 .. -DCMAKE_INSTALL_PREFIX=${sse41_prefix} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=ON \
  -DGMX_FFT_LIBRARY=mkl \
  -DGMX_CPU_ACCELERATION=SSE4.1 \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
setenv CC mpiicc
setenv CXX mpiicpc
setenv F77 mpiifort
setenv F90 mpiifort
setenv FC mpiifort
mkdir rccs-mpi
cd rccs-mpi
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=ON \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=OFF \
  -DGMX_FFT_LIBRARY=mkl \
  -DMPICH=/opt/intel/impi/4.1.3.049/intel64/bin/mpirun \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
mkdir rccs-mpi-d
cd rccs-mpi-d
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=ON \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=ON \
  -DGMX_FFT_LIBRARY=mkl \
  -DMPICH=/opt/intel/impi/4.1.3.049/intel64/bin/mpirun \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
mkdir rccs-mpi-d-sse41
cd rccs-mpi-d-sse41
cmake28 .. -DCMAKE_INSTALL_PREFIX=${sse41_prefix} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=ON \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=ON \
  -DGMX_FFT_LIBRARY=mkl \
  -DGMX_CPU_ACCELERATION=SSE4.1 \
  -DMPICH=/opt/intel/impi/4.1.3.049/intel64/bin/mpirun \

```

```
-DREGRESSIONTEST_DOWNLOAD=OFF  
make -j 12  
make install  
cd ..
```