

Gromacs 4.6.5 for UV2000

Webpage

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

Version

Gromacs 4.6.5

Tools for Compiling

- Intel Compiler 14.0.2
- MPT 2.0.7
- 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/uv/gromacs465
set sse41_prefix=/local/apl/uv/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 ${file_gromacs}
cd gromacs-4.6.5
#
setenv CC icc
setenv CXX icpc
setenv F77 ifort
setenv F90 ifort
setenv FC ifort
mkdir rccs
cd rccs
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=OFF \
  -DGMX_FFT_LIBRARY=mkl \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make VERBOSE=1 -j 12
make install
cd ..
#
mkdir rccs-d
cd rccs-d
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=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
cmake .. -DCMAKE_INSTALL_PREFIX=${sse41_prefix} \
-DMAKE_VERBOSE_MAKEFILE=ON \
-DGMX_MPI=OFF \
-DGMX_GPU=OFF \
-DGMX_DOUBLE=ON \
-DGMX_FFT_LIBRARY=mkl \
-DGMX_CPU_ACCELERATION=SSE4.1 \
-DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
setenv CC mpicc
setenv CXX mpicxx
setenv F77 mpif90
setenv F90 mpif90
setenv FC mpif90
mkdir rccs-mpi
cd rccs-mpi
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix} \
-DMAKE_VERBOSE_MAKEFILE=ON \
-DGMX_MPI=ON \
-DGMX_GPU=OFF \
-DGMX_DOUBLE=OFF \
-DGMX_FFT_LIBRARY=mkl \
-DMPIEXEC=/opt/sji/mpt/mpt-2.07/bin/mpirun \
-DREGRESSIONTEST_DOWNLOAD=OFF
make VERBOSE=1 -j 12
make install
cd ..
#
mkdir rccs-mpi-d
cd rccs-mpi-d
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix} \
-DMAKE_VERBOSE_MAKEFILE=ON \
-DGMX_MPI=ON \
-DGMX_GPU=OFF \
-DGMX_DOUBLE=ON \
-DGMX_FFT_LIBRARY=mkl \
-DMPIEXEC=/opt/sji/mpt/mpt-2.07/bin/mpirun \
-DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
mkdir rccs-mpi-d-sse41
cd rccs-mpi-d
cmake .. -DCMAKE_INSTALL_PREFIX=${sse41_prefix} \
-DMAKE_VERBOSE_MAKEFILE=ON \
-DGMX_MPI=ON \
-DGMX_GPU=OFF \
-DGMX_DOUBLE=ON \
-DGMX_FFT_LIBRARY=mkl \
-DGMX_CPU_ACCELERATION=SSE4.1 \
-DMPIEXEC=/opt/sji/mpt/mpt-2.07/bin/mpirun \
-DREGRESSIONTEST_DOWNLOAD=OFF

```

```
make -j 12  
make install  
cd ..
```