

Gromacs 4.6.6 for UV2000

Webpage

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

Version

Gromacs 4.6.6

Tools for Compiling

- Intel Compiler 13.1.1
- MPT 2.0.7
- cmake 2.8.11

Necessary Files for Compiling

- gromacs-4.6.6.tar.gz
- [no-gcc-version.patch](#)

Patch Files

no-gcc-version.patch

```
--- cmake/gmxManageNvccConfig.cmake.orig 2014-06-20 21:17:13.000000000 +0900
+++ cmake/gmxManageNvccConfig.cmake 2014-07-17 08:52:24.341434579 +0900
@@ -109,16 +109,16 @@
     # as even with icc use as host compiler, when icc's gcc compatibility
     # mode is higher than the max gcc version officially supported by CUDA,
     # nvcc will freak out.
-   if (UNIX AND CMAKE_C_COMPILER_ID MATCHES "Intel" AND
-       CUDA_HOST_COMPILER_AUTOSET)
-       if (CUDA_VERSION VERSION_LESS "4.1")
-           message(STATUS "Setting Intel Compiler compatibity mode to gcc 4.4 for nvcc host compilation")
-           set(CUDA_HOST_COMPILER_OPTIONS "${CUDA_HOST_COMPILER_OPTIONS};-Xcompiler;-gcc-version=440;")
-       else()
-           message(STATUS "Setting Intel Compiler compatibity mode to gcc 4.5 for nvcc host compilation")
-           set(CUDA_HOST_COMPILER_OPTIONS "${CUDA_HOST_COMPILER_OPTIONS};-Xcompiler;-gcc-version=450;")
-       endif()
-   endif()
+#   if (UNIX AND CMAKE_C_COMPILER_ID MATCHES "Intel" AND
+#       CUDA_HOST_COMPILER_AUTOSET)
+#       if (CUDA_VERSION VERSION_LESS "4.1")
+#           message(STATUS "Setting Intel Compiler compatibity mode to gcc 4.4 for nvcc host compilation")
+#           set(CUDA_HOST_COMPILER_OPTIONS "${CUDA_HOST_COMPILER_OPTIONS};-Xcompiler;-gcc-version=440;")
+#       else()
+#           message(STATUS "Setting Intel Compiler compatibity mode to gcc 4.5 for nvcc host compilation")
+#           set(CUDA_HOST_COMPILER_OPTIONS "${CUDA_HOST_COMPILER_OPTIONS};-Xcompiler;-gcc-version=450;")
+#       endif()
+#   endif()
    set(CUDA_HOST_COMPILER_OPTIONS "${CUDA_HOST_COMPILER_OPTIONS}"
        CACHE STRING "Options for nvcc host compiler (do not edit!)." FORCE)
```

Attention

Setting `GMX_CPU_ACCELERATION=AVX_256` makes two fails in freeenergy of regressiontests.
So, need preparation of SSE4.1 binary files.

Procedure of Compiling

```

#!/bin/csh -f
umask 022
set file_gromacs=/home/users/${USER}/build/gromacs466/gromacs-4.6.6.tar.gz
set file_patch1=/home/users/${USER}/build/gromacs466/no-gcc-version.patch
set work=/work/users/${USER}
set prefix_avx256=/local/apl/uv/gromacs466
set prefix_sse41=/local/apl/uv/gromacs466_sse41
source /opt/intel/composer_xe_2013.3.163/bin/compilervars.csh intel64
#-----
cd ${work}
if (-d gromacs-4.6.6) then
  mv gromacs-4.6.6 gromacs-4.6.6-erase
  rm -rf gromacs-4.6.6-erase &
endif
tar xzf ${file_gromacs}
cd gromacs-4.6.6
patch -p0 < ${file_patch1}
#
setenv CC icc
setenv CXX icpc
setenv F77 ifort
setenv F90 ifort
setenv FC ifort
mkdir rccs
cd rccs
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix_avx256} \
  -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=${prefix_avx256} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=ON \
  -DGMX_FFT_LIBRARY=mkl \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
mkdir rccs-sse41
cd rccs-sse41
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix_sse41} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=OFF \
  -DGMX_FFT_LIBRARY=mkl \
  -DGMX_CPU_ACCELERATION=SSE4.1 \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make VERBOSE=1 -j 12
make install
cd ..
#
mkdir rccs-d-sse41
cd rccs-d-sse41

```

```

cmake .. -DCMAKE_INSTALL_PREFIX=${prefix_sse41} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=OFF \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=ON \
  -DGMX_FFT_LIBRARY=mkl \
  -DGMX_CPU_ACCELERATION=SSE4.1 \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
setenv CC mpicc
setenv CXX mpicxx
setenv F77 mpif90
setenv F90 mpif90
setenv FC mpif90
mkdir rccs-mpi
cd rccs-mpi
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix_avx256} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=ON \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=OFF \
  -DGMX_FFT_LIBRARY=mkl \
  -DMPICH=/opt/sgi/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=${prefix_avx256} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=ON \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=ON \
  -DGMX_FFT_LIBRARY=mkl \
  -DMPICH=/opt/sgi/mpt/mpt-2.07/bin/mpirun \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
mkdir rccs-mpi-sse41
cd rccs-mpi-sse41
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix_sse41} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=ON \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=OFF \
  -DGMX_FFT_LIBRARY=mkl \
  -DGMX_CPU_ACCELERATION=SSE4.1 \
  -DMPICH=/opt/sgi/mpt/mpt-2.07/bin/mpirun \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make VERBOSE=1 -j 12
make install
cd ..
#
mkdir rccs-mpi-d-sse41
cd rccs-mpi-d-sse41
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix_sse41} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=ON \

```

```
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=ON \  
-DGMX_FFT_LIBRARY=mkl \  
-DGMX_CPU_ACCELERATION=SSE4.1 \  
-DMPIEXEC=/opt/sgj/mpt/mpt-2.07/bin/mpirun \  
-DREGRESSIONTEST_DOWNLOAD=OFF  
make -j 12  
make install  
cd ..
```