

Gromacs 5.0 for UV2000

Webpage

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

Version

5.0

Tools for Compiling

- Intel Compiler 13.1.1
- MPT 2.0.7
- cmake 2.8.11

Necessary Files for Compiling

- gromacs-5.0.tar.gz
- [no-gcc-version.patch](#)
- [no-mpifinalized.patch](#)

Patch Files

no-gcc-version.patch

```
--- cmake/gmxManageNvccConfig.cmake.orig 2014-07-09 09:43:31.108489646 +0900
+++ cmake/gmxManageNvccConfig.cmake      2014-07-09 09:44:24.668688300 +0900
@@ -109,16 +109,16 @@
     # as even with icc used 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)
```

no-mpifinalized.patch

```

--- src/gromacs/utility/init.cpp.orig 2014-07-10 11:07:50.617514888 +0900
+++ src/gromacs/utility/init.cpp      2014-07-10 11:09:20.845939159 +0900
@@ -67,8 +67,6 @@
{
#ifdef GMX_LIB_MPI
    int isInitialized = 0, isFinalized = 0;
-   MPI_Finalized(&isFinalized);
-   GMX_RELEASE_ASSERT(!isFinalized, "Invalid attempt to initialize MPI after finalization");
    MPI_Initialized(&isInitialized);
    if (isInitialized)
    {

```

Attention

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

Procedure of Compiling

```

#!/bin/csh -f
umask 022
set file_gromacs=/home/users/${USER}/build/gromacs500/gromacs-5.0.tar.gz
set file_patch1=/home/users/${USER}/build/gromacs500/no-gcc-version.patch
set file_patch3=/home/users/${USER}/build/gromacs500/no-mpifinalized.patch
set prefix_avx256=/local/apl/uv/gromacs500
set prefix_sse41=/local/apl/uv/gromacs500_sse41
set work=/work/users/${USER}
source /opt/intel/composer_xe_2013.3.163/bin/compilervars.csh intel64
#-----
cd ${work}
if (-d gromacs-5.0) then
    mv gromacs-5.0 gromacs-erase
    rm -rf gromacs-erase &
endif
tar xzf ${file_gromacs}
cd gromacs-5.0
patch -p0 < ${file_patch1}
patch -p0 < ${file_patch3}
#
setenv CC icc
setenv CXX icpc
setenv F77 ifort
setenv F90 ifort
setenv FC ifort
mkdir rccs-s
cd rccs-s
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix_avx256} \
    -DCMAKE_VERBOSE_MAKEFILE=ON \
    -DGMX_MPI=OFF \
    -DGMX_GPU=OFF \
    -DGMX_DOUBLE=OFF \
    -DGMX_FFT_LIBRARY=mkl \
    -DGMX_SYMLINK_OLD_BINARY_NAMES=OFF \
    -DREGRESSIONTEST_DOWNLOAD=OFF
make -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_GPU=OFF \
-DGMX_DOUBLE=ON \
-DGMX_FFT_LIBRARY=mkl \
-DGMX_SYMLINK_OLD_BINARY_NAMES=OFF \
-DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
mkdir rccs-s-sse41
cd rccs-s-sse41
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix_sse41} \
-DMAKE_VERBOSE_MAKEFILE=ON \
-DGMX_MPI=OFF \
-DGMX_GPU=OFF \
-DGMX_DOUBLE=OFF \
-DGMX_FFT_LIBRARY=mkl \
-DGMX_CPU_ACCELERATION=SSE4.1 \
-DGMX_SYMLINK_OLD_BINARY_NAMES=OFF \
-DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
mkdir rccs-d-sse41
cd rccs-d-sse41
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix_sse41} \
-DMAKE_VERBOSE_MAKEFILE=ON \
-DGMX_MPI=OFF \
-DGMX_GPU=OFF \
-DGMX_DOUBLE=ON \
-DGMX_FFT_LIBRARY=mkl \
-DGMX_CPU_ACCELERATION=SSE4.1 \
-DGMX_SYMLINK_OLD_BINARY_NAMES=OFF \
-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=${prefix_avx256} \
-DMAKE_VERBOSE_MAKEFILE=ON \
-DGMX_MPI=ON \
-DGMX_GPU=OFF \
-DGMX_DOUBLE=OFF \
-DGMX_FFT_LIBRARY=mkl \
-DMPIEXEC=/opt/sji/mpt/mpt-2.07/bin/mpirun \
-DGMX_SYMLINK_OLD_BINARY_NAMES=OFF \
-DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
mkdir rccs-mpi-d
cd rccs-mpi-d
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix_avx256} \
-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 \  
-DGMX_SYMLINK_OLD_BINARY_NAMES=OFF \  
-DREGRESSIONTEST_DOWNLOAD=OFF  
make -j 12  
make install  
cd ..  
mkdir rccs-mpi-sse41  
cd rccs-mpi-sse41  
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix_sse41} \  
-DCMAKE_VERBOSE_MAKEFILE=ON \  
-DGMX_MPI=ON \  
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=OFF \  
-DGMX_FFT_LIBRARY=mkl \  
-DGMX_CPU_ACCELERATION=SSE4.1 \  
-DMPIEXEC=/opt/sji/mpt/mpt-2.07/bin/mpirun \  
-DGMX_SYMLINK_OLD_BINARY_NAMES=OFF \  
-DREGRESSIONTEST_DOWNLOAD=OFF  
make -j 12  
make install  
cd ..  
#  
mkdir rccs-mpi-d-sse41  
cd rccs-mpi-d-sse41  
cmake .. -DCMAKE_INSTALL_PREFIX=${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/sji/mpt/mpt-2.07/bin/mpirun \  
-DGMX_SYMLINK_OLD_BINARY_NAMES=OFF \  
-DREGRESSIONTEST_DOWNLOAD=OFF  
make -j 12  
make install  
cd ..
```