Gromacs 5.0 for Primargy RX300/CX250

Webpage

http://www.gromacs.org/

Version

5.0

Tools for Compiling

- Intel Compiler 13.1.1
- Cuda compilation tools, release 5.0, V0.2.1221
- Intel MPI 4.1.0.030
- cmake 2.8.8

Necessary Files for Compiling

- gromacs-5.0.tar.gz
- no-gcc-version.patch
- int128.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)
```

int128.patch

```
--- src/external/boost/boost/config/compiler/intel.hpp.orig    2014-06-18 00:14:19.000000000 +0900
+++ src/external/boost/boost/config/compiler/intel.hpp    2014-07-09 09:59:27.000000000 +0900
@@ -35,10 +35,14 @@
 #endif

 #ifdef BOOST_INTEL_STDCXX0X
+#ifndef BOOST_COMPILER
 #define BOOST_COMPILER "Intel C++ C++0x mode version " BOOST_STRINGIZE(BOOST_INTEL_CXX_VERSION)
+#endif
 #else
+#ifndef BOOST_COMPILER
 #define BOOST_COMPILER "Intel C++ version " BOOST_STRINGIZE(BOOST_INTEL_CXX_VERSION)
 #endif
+#endif
 #define BOOST_INTEL BOOST_INTEL_CXX_VERSION

 #if defined(_WIN32) || defined(_WIN64)
@@ -303,10 +307,6 @@
 #  define BOOST_HAS_STDINT_H
 #endif

-#if defined(__LP64__) && defined(__GNUC__) && (BOOST_INTEL_CXX_VERSION >= 1310)
-#  define BOOST_HAS_INT128
-#endif
-
 //
 // last known and checked version:
 #if (BOOST_INTEL_CXX_VERSION > 1310)
```

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/${USER}/build/gromacs500/gromacs-5.0.tar.gz
set file_patch1=/home/users/${USER}/build/gromacs500/no-gcc-version.patch
set file_patch2=/home/users/${USER}/build/gromacs500/int128.patch
set prefix_avx256=/local/apl/pg/gromacs500
set prefix_sse41=/local/apl/pg/gromacs500_sse41
set work=/work/users/${USER}
#------------------------------------------------------------------------------
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 < ${file_patch2}
#
setenv CC icc
setenv CXX icpc
setenv F77 ifort
setenv F90 ifort
setenv FC ifort
mkdir rccs-gpu
cd rccs-gpu
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix_avx256} \
        -DCMAKE_VERBOSE_MAKEFILE=ON \
```

```
        -DCMAKE_VERBOSE_MAKEFILE=ON \
        -DGMX_MPI=OFF \
        -DGMX_GPU=ON \
        -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
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix_avx256} \
        -DCMAKE_VERBOSE_MAKEFILE=ON \
        -DGMX_MPI=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-gpu-sse41
cd rccs-gpu-sse41
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix_sse41} \
        -DCMAKE_VERBOSE_MAKEFILE=ON \
        -DGMX_MPI=OFF \
        -DGMX_GPU=ON \
        -DGMX_DOUBLE=OFF \
        -DGMX_FFT_LIBRARY=mkl \
        -DGMX_CPU_ACCELERATION=SSE4.1 \
        -DGMX_SYMLINK_OLD_BINARY_NAMES=OFF \
        -DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
mkdir rccs-d-sse41
cd rccs-d-sse41
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix_sse41} \
        -DCMAKE_VERBOSE_MAKEFILE=ON \
        -DGMX_MPI=OFF \
        -DGMX_GPU=OFF \
        -DGMX_DOUBLE=ON \
        -DGMX_FFT_LIBRARY=mkl \
        -DGMX_CPU_ACCELERATION=SSE4.1 \
        -DGMX_SYMLINK_OLD_BINARY_NAMES=OFF \
        -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_avx256} \
        -DCMAKE_VERBOSE_MAKEFILE=ON \
        -DGMX_MPI=ON \
        -DGMX_GPU=OFF \
```

```
        -DGMX_DOUBLE=OFF \
        -DGMX_FFT_LIBRARY=mkl \
        -DMPIEXEC=/opt/intel/impi/4.1.0.030/intel64/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
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix_avx256} \
        -DCMAKE_VERBOSE_MAKEFILE=ON \
        -DGMX_MPI=ON \
        -DGMX_GPU=OFF \
        -DGMX_DOUBLE=ON \
        -DGMX_FFT_LIBRARY=mkl \
        -DMPIEXEC=/opt/intel/impi/4.1.0.030/intel64/bin/mpirun \
        -DGMX_SYMLINK_OLD_BINARY_NAMES=OFF \
        -DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
mkdir rccs-mpi-sse41
cd rccs-mpi-sse41
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix_sse41} \
        -DCMAKE_VERBOSE_MAKEFILE=ON \
        -DGMX_MPI=ON \
        -DGMX_GPU=OFF \
        -DGMX_DOUBLE=OFF \
        -DGMX_FFT_LIBRARY=mkl \
        -DMPIEXEC=/opt/intel/impi/4.1.0.030/intel64/bin/mpirun \
        -DGMX_CPU_ACCELERATION=SSE4.1 \
        -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
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix_sse41} \
        -DCMAKE_VERBOSE_MAKEFILE=ON \
        -DGMX_MPI=ON \
        -DGMX_GPU=OFF \
        -DGMX_DOUBLE=ON \
        -DGMX_FFT_LIBRARY=mkl \
        -DMPIEXEC=/opt/intel/impi/4.1.0.030/intel64/bin/mpirun \
        -DGMX_CPU_ACCELERATION=SSE4.1 \
        -DGMX_SYMLINK_OLD_BINARY_NAMES=OFF \
        -DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
```