

Gromacs 5.1.2 for GPU

Webpage

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

Version

5.1.2

Tools for Compiling

- ▶ Intel Compiler 15.0.2
- ▶ Cuda compilation tools, release 7.5, V7.5.17
- ▶ cmake 2.8.8

Necessary Files for Compiling

- ▶ gromacs-5.1.2.tar.gz
- ▶ [int128.patch](#)

Patch Files

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
```

Procedure of Compiling

```
#!/bin/csh -f
umask 022
set file_gromacs=/home/users/${USER}/build/gromacs512/gromacs-5.1.2.tar.gz
set file_patch2=/home/users/${USER}/build/gromacs512/int128.patch
set prefix=/local/apl/pg/gromacs512-CUDA
#set work=/work/users/${USER}
set work=/dev/shm/${USER}
source /opt/intel/composer_xe_2015.2.164/bin/compilervars.csh intel64
#-----
cd ${work}
if (-d gromacs-5.1.2) then
  mv gromacs-5.1.2 gromacs-erase
  rm -rf gromacs-erase &
endif
tar xzf ${file_gromacs}
cd gromacs-5.1.2
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} \
-DMAKE_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 ..
```
