

Gromacs 5.1.2 for Primargy

Webpage

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

Version

5.1.2

Tools for Compiling

- Intel Compiler 15.0.2
- Intel MPI 5.0.3.048
- 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
set work=/work/users/${USER}
source /opt/intel/composer_xe_2015.2.164/bin/compilervars.csh intel64
```

```
source /opt/intel/composer_xe_2019.2.104/bin/compilervars.sh 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 < ${file_patch2}  
#  
setenv CC icc  
setenv CXX icpc  
setenv F77 ifort  
setenv F90 ifort  
setenv FC ifort  
mkdir rccs-s  
cd rccs-s  
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix} \  
  -DCMAKE_VERBOSE_MAKEFILE=ON \  
  -DGMX_MPI=OFF \  
  -DGMX_GPU=OFF \  
  -DGMX_DOUBLE=OFF \  
  -DGMX_THREAD_MPI=OFF \  
  -DGMX_FFT_LIBRARY=mkl \  
  -DREGRESSIONTEST_DOWNLOAD=OFF  
make -j 12  
make install  
cd ..  
#  
mkdir rccs-d  
cd rccs-d  
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix} \  
  -DCMAKE_VERBOSE_MAKEFILE=ON \  
  -DGMX_MPI=OFF \  
  -DGMX_GPU=OFF \  
  -DGMX_DOUBLE=ON \  
  -DGMX_THREAD_MPI=OFF \  
  -DGMX_FFT_LIBRARY=mkl \  
  -DREGRESSIONTEST_DOWNLOAD=OFF  
make -j 12  
make install  
cd ..  
#  
setenv CC mpiicc  
setenv CXX mpiicpc  
setenv F77 mpiifort  
setenv F90 mpiifort  
setenv FC mpiifort  
mkdir rccs-mpi  
cd rccs-mpi  
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix} \  
  -DCMAKE_VERBOSE_MAKEFILE=ON \  
  -DGMX_MPI=ON \  
  -DGMX_GPU=OFF \  
  -DGMX_DOUBLE=OFF \  
  -DGMX_THREAD_MPI=OFF \  
  -DGMX_FFT_LIBRARY=mkl \  
  -DMPICH_CXX=/opt/intel/impi/5.0.3.048/intel64/bin/mpirun \  
  -DREGRESSIONTEST_DOWNLOAD=OFF  
make -j 12  
make install  
cd ..  
#  
mkdir rccs-mpi-d  
cd rccs-mpi-d
```

```
cmake28 .. -DCMAKE_INSTALL_PREFIX=${prefix} \  
-DCMAKE_VERBOSE_MAKEFILE=ON \  
-DGMX_MPI=ON \  
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=ON \  
-DGMX_THREAD_MPI=OFF \  
-DGMX_FFT_LIBRARY=mkl \  
-DMPIEXEC=/opt/intel/impi/5.0.3.048/intel64/bin/mpirun \  
-DREGRESSIONTEST_DOWNLOAD=OFF  
make -j 12  
make install  
cd ..
```