

Gromacs 5.1.2 for UV2000

Webpage

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

Version

5.1.2

Tools for Compiling

- ▶ Intel Compiler 15.0.2
- ▶ MPT 2.11
- ▶ cmake 2.8.11

Necessary Files for Compiling

- ▶ [gromacs-5.1.2.tar.gz](#)
- ▶ [no-mpifinalized.patch](#)

Patch Files

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)
     {
```

Procedure of Compiling

```
#!/bin/csh -f
umask 022

set file_gromacs=/home/users/${USER}/build/gromacs512/gromacs-5.1.2.tar.gz
set file_patch3=/home/users/${USER}/build/gromacs512/no-mpifinalized.patch
set prefix=/local/apl/uv/gromacs512
set work=/work/users/${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 < ${file_patch3}
#
setenv CC icc
setenv CXX icpc
setenv F77 ifort
setenv F90 ifort
setenv FC ifort
mkdir rccs-s
cd rccs-s
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix} \
    -DCMAKE_VERBOSE_MAKEFILE=ON \
    -DGMX_MPI=OFF \
    -DGMX_THREAD_MPI=OFF \
    -DGMX_GPU=OFF \
    -DGMX_DOUBLE=OFF \
    -DGMX_FFT_LIBRARY=mkl \
    -DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
mkdir rccs-d
cd rccs-d
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix} \
```

```
-DCMAKE_VERBOSE_MAKEFILE=ON \  
-DGMX_MPI=OFF \  
-DGMX_THREAD_MPI=OFF \  
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=ON \  
-DGMX_FFT_LIBRARY=mkl \  
-DREGRESSIONTEST_DOWNLOAD=OFF  
make -j 12  
make install  
cd ..  
#  
#  
setenv CC mpicc  
setenv CXX mpicxx  
setenv F77 mpi90  
setenv F90 mpi90  
setenv FC mpi90  
mkdir rccs-mpi  
cd rccs-mpi  
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix} \  
-DCMAKE_VERBOSE_MAKEFILE=ON \  
-DGMX_MPI=ON \  
-DGMX_THREAD_MPI=OFF \  
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=OFF \  
-DGMX_FFT_LIBRARY=mkl \  
-DMPIEXEC=/opt/sgi/mpt/mpt-2.11/bin/mpirun \  
-DREGRESSIONTEST_DOWNLOAD=OFF  
make -j 12  
make install  
cd ..  
#  
#  
mkdir rccs-mpi-d  
cd rccs-mpi-d  
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix} \  
-DCMAKE_VERBOSE_MAKEFILE=ON \  
-DGMX_MPI=ON \  
-DGMX_THREAD_MPI=OFF \  
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=ON \  
-DGMX_FFT_LIBRARY=mkl \  
-DMPIEXEC=/opt/sgi/mpt/mpt-2.11/bin/mpirun \  
-DREGRESSIONTEST_DOWNLOAD=OFF  
make -j 12  
make install  
cd ..
```
