

## 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
```

```
cd rccs-d
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 mpif90
setenv F90 mpif90
setenv FC mpif90
mkdir rccs-mpi
cd rccs-mpi
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=ON \
  -DGMX_THREAD_MPI=OFF \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=OFF \
  -DGMX_FFT_LIBRARY=mkl \
  -DMPICH=/opt/sji/mpt/mpt-2.11/bin/mpirun \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
#
mkdir rccs-mpi-d
cd rccs-mpi-d
cmake .. -DCMAKE_INSTALL_PREFIX=${prefix} \
  -DCMAKE_VERBOSE_MAKEFILE=ON \
  -DGMX_MPI=ON \
  -DGMX_THREAD_MPI=OFF \
  -DGMX_GPU=OFF \
  -DGMX_DOUBLE=ON \
  -DGMX_FFT_LIBRARY=mkl \
  -DMPICH=/opt/sji/mpt/mpt-2.11/bin/mpirun \
  -DREGRESSIONTEST_DOWNLOAD=OFF
make -j 12
make install
cd ..
```