

## Gromacs 5.1.4 for UV2000

### Webpage

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

### Version

5.1.4

### Tools for Compiling

- Intel Compiler 16.0.2
- MPT 2.13
- cmake 2.8.11

### Necessary Files for Compiling

- gromacs-5.1.4.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/${USER}/build/gromacs514/gromacs-5.1.4.tar.gz
set file_patch3=/home/users/${USER}/build/gromacs514/no-mpifinalized.patch
set prefix=/local/apl/uv/gromacs514
set work=/work/users/${USER}
#-----
cd ${work}
if (-d gromacs-5.1.4) then
    mv gromacs-5.1.4 gromacs-erase
    rm -rf gromacs-erase &
endif
tar xzf ${file_gromacs}
cd gromacs-5.1.4
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} \
```

```
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=${prefix} \  
-DCMAKE_VERBOSE_MAKEFILE=ON \  
-DGMX_MPI=ON \  
-DGMX_THREAD_MPI=OFF \  
-DGMX_GPU=OFF \  
-DGMX_DOUBLE=OFF \  
-DGMX_FFT_LIBRARY=mkl \  
-DMPICH=/opt/sji/mpt/mpt-2.13/bin/mpirun \  
-DREGRESSIONTEST_DOWNLOAD=OFF  
make -j 12  
make install  
cd ..  
#  
mkdir rccs-mpi-d  
cd rccs-mpi-d  
cmake .. -DCMAKE_INSTALL_PREFIX=${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-2.13/bin/mpirun \  
-DREGRESSIONTEST_DOWNLOAD=OFF  
make -j 12  
make install  
cd ..
```