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// Building the QXMD software on the Discovery cluster
// First, clone the QXMD GitHub repository
[anakano@discovery1 ~]$ mkdir qxmd
[anakano@discovery1 ~]$ cd qxmd
[anakano@discovery1 qxmd]$ git clone https://github.com/USCCACS/QXMD_DEV.git
Cloning into 'QXMD_DEV'...
Username for 'https://github.com': aiichironakano
Password for 'https://aiichironakano@github.com':
...
Checking out files: 100% (657/657), done.
// Load the necessary software modules & prepare for make using the cmake command
[anakano@discovery1 qxmd]$ cd QXMD_DEV
[anakano@discovery1 QXMD_DEV]$ module purge
[anakano@discovery1 QXMD_DEV]$ module load usc
[anakano@discovery1 QXMD_DEV]$ module load cmake
[anakano@discovery1 QXMD_DEV]$ module load fftw
[anakano@discovery1 QXMD_DEV]$ mkdir build
[anakano@discovery1 QXMD_DEV]$ cd build
[anakano@discovery1 build]$ cmake -DCMAKE_Fortran_COMPILER=mpif90 ..
-- The Fortran compiler identification is GNU 11.3.0
...
-- Build files have been written to: /home1/anakano/qxmd/QXMD_DEV/build
// Build the qxmd software using the make command with 8 threads
[anakano@discovery1 build]$ make -j8
Scanning dependencies of target mpi_wrapper
Scanning dependencies of target qxmd_lib
[ 1%] Building Fortran object Sources/CMakeFiles/mpi_wrapper.dir/mpi_comm.f90.o
...
[100%] Built target qxmd_exe
// The executable named qxmd is now in the build/bin directory
[anakano@discovery1 build]$ cd bin
[anakano@discovery1 bin]$ pwd
/home1/anakano/qxmd/QXMD_DEV/build/bin
[anakano@discovery1 bin]$ ls
qxmd
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