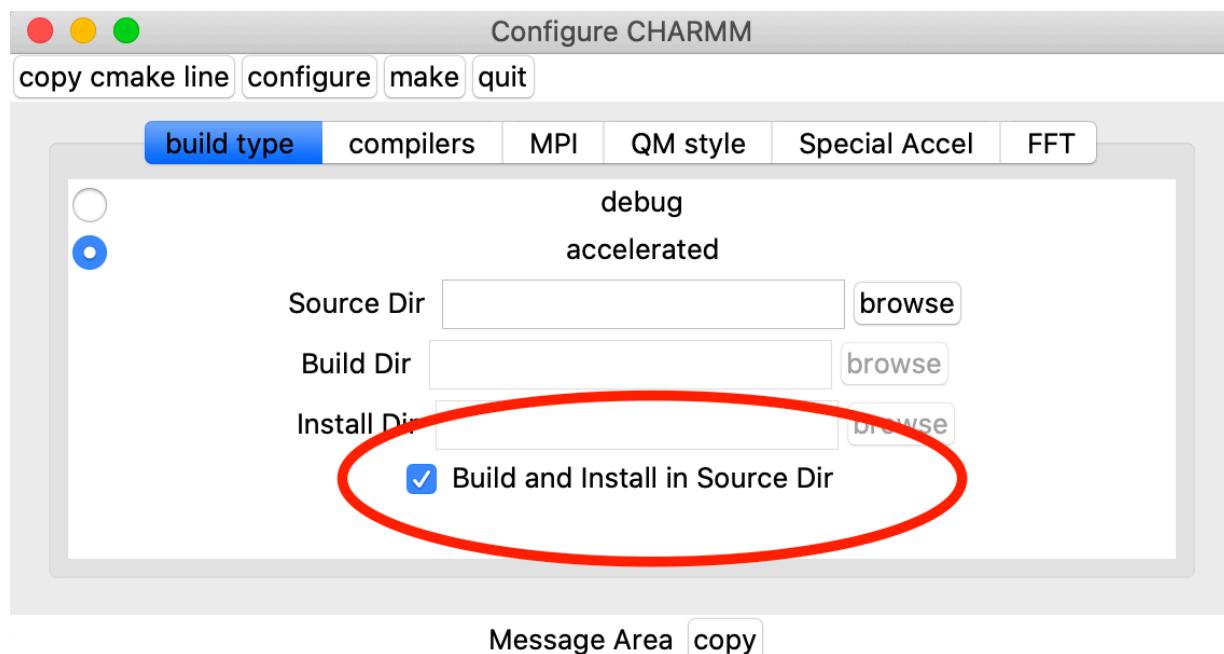


How to use config.py

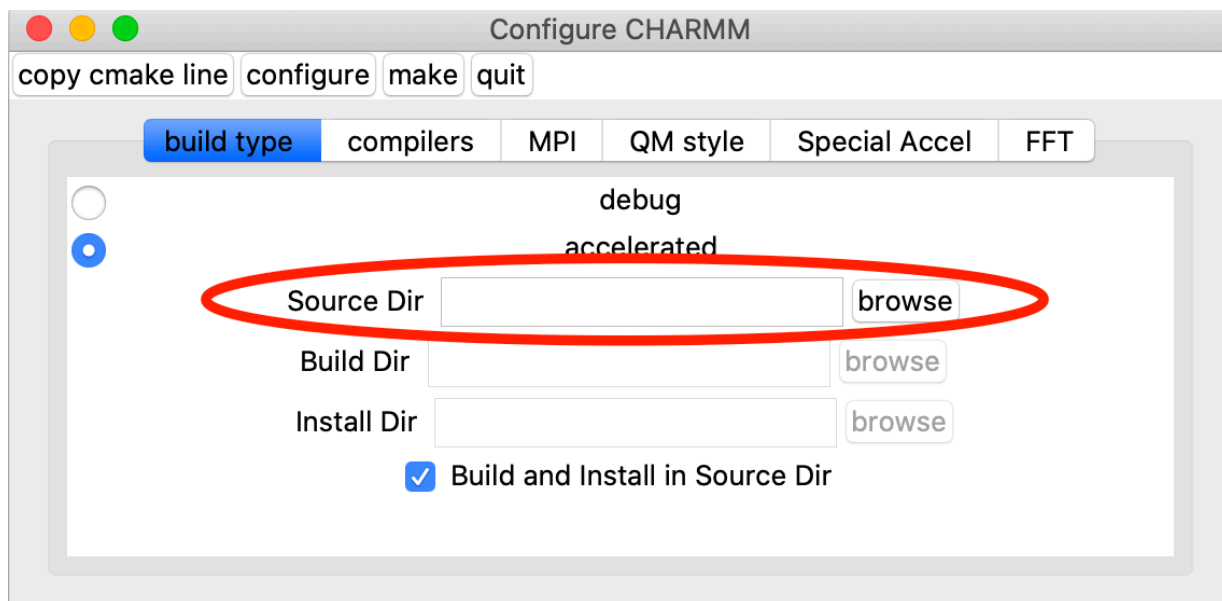
In-place install

An in-place install creates the build, lib, and bin directories as subdirectories of the CHARMM source directory.

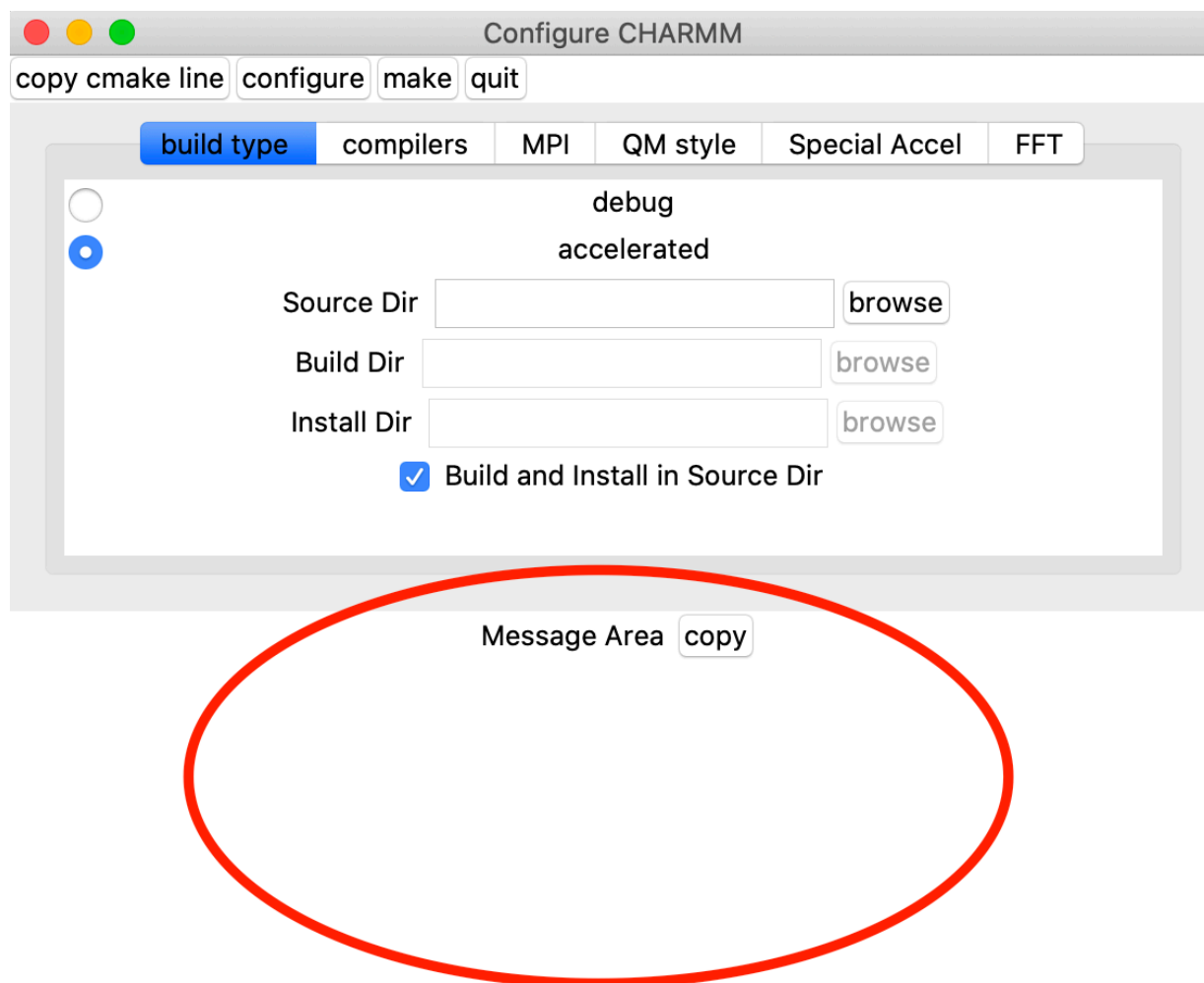
1. In the 'build type' tab, make sure the box labeled 'Build and Install in Source Dir' is checked.



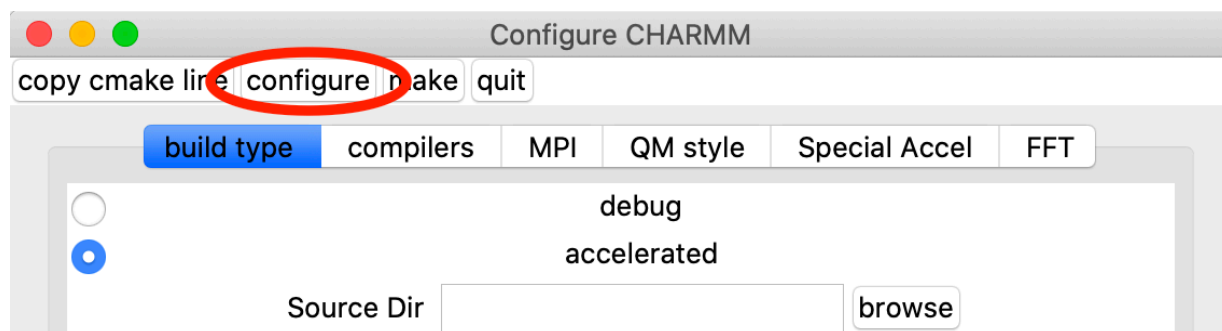
2. In the 'build type' tab, browse to or type the path of the CHARMM source directory in the entry labeled 'Source Dir'.



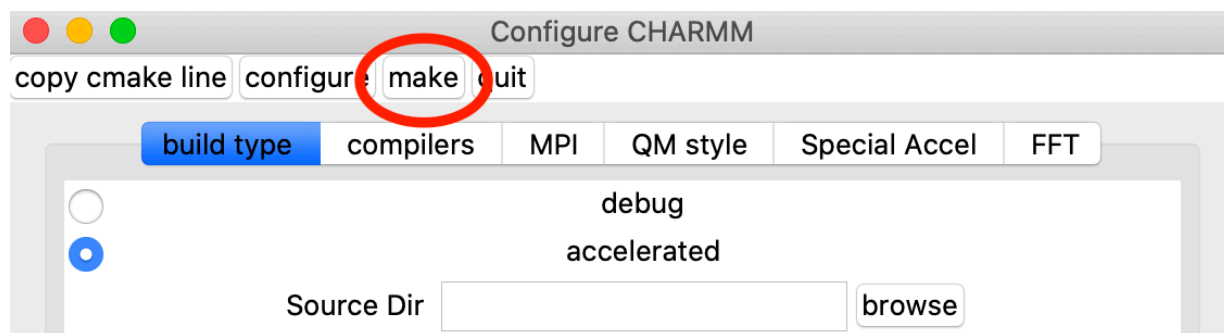
3. Select or deselect the other options from the other tabs or entries that you'd like. It is ok to leave some entries blank. CMake will attempt to find sane default values. Any errors will be displayed in the 'Message Area' after the 'configure' and 'make' buttons are pressed.



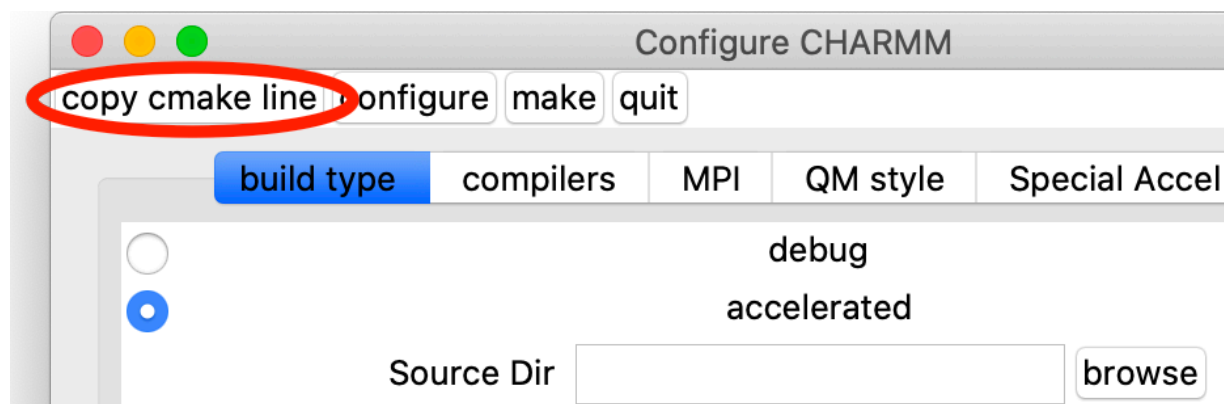
4. Press the 'configure' button.



5. Press the 'make' button.



6. As an alternative to Steps 4 and 5, you may press the 'copy cmake line' button. Then the appropriate cmake command line will be copied to your system's clipboard and you can paste it into a terminal emulator.



Out-of-source install

If you need to use different directories to build and install CHARMM, uncheck the box labeled 'Build and Install in Source Dir' and fill in the 'Source Dir' and 'Build Dir' entries.

Configure CHARMM

copy cmake line configure make quit

build type compilers MPI QM style Special Accel FFT

debug
accelerated

Source Dir browse

Build Dir browse

Install Dir browse

☒ Build and Install in Source Dir

Message Area