Quantum Espresso – Download and Compilation Instructions

For WINDOWS (i.e. Ubuntu via WSL):

1. Download QE V.7.2 from: <https://www.quantum-espresso.org/download-page/>
   1. NOTE: You will be asked to register an account. This is free and should require minimal setup.
2. Copy the downloaded “qe-7.2-ReleasePack.tar.gz” file to your SOFTWARE directory (or wherever you would like to install)
3. Untar with the following: tar -xzvf qe-7.2-ReleasePack.tar.gz
4. Change to the qe-7.2 directory (i.e. cd qe-7.2)
5. Perform the following commands:
   1. sudo apt-get update
   2. sudo apt-get upgrade
   3. sudo apt install git
   4. sudo apt install gcc
   5. sudo apt install gfortran
   6. sudo apt install libfftw3-dev
   7. sudo apt install make
6. Now we should be set to compile the software with the following:
   1. ./configure
   2. make all

For MacOS:

1. Download QE V.7.2 from: <https://www.quantum-espresso.org/download-page/>
   1. NOTE: You will be asked to register an account. This is free and should require minimal setup.
2. Copy the downloaded “qe-7.2-ReleasePack.tar.gz” file to your SOFTWARE directory (or wherever you would like to install)
3. Untar with the following: tar -xzvf qe-7.2-ReleasePack.tar.gz
4. Change to the qe-7.2 directory (i.e. cd qe-7.2)
5. Try compiling. Your system already has the appropriate libraries.
   1. ./configure
   2. make all
6. If this resulted in any errors, fret not! We will troubleshoot together!