How to Configure Quantum Espresso on JHU-MARCC

Step 1: Customize the 'Unix shell' environment

We can customize the 'Unix shell' environment by adding modules that we will need later on. Copy/paste the following exactly as it is into the terminal:

```
$ cat >> .bashrc << EOF
module load fftw3/3.3.8
module load xcrysden
module load gnuplot/4.6.2
module load openmpi/3.1
EOF
source ~/.bashrc
```

Step 2: Download QE

In order to use QE, download the latest version of the package from https://gitlab.com/QEF/q-e/tags and install it in your working directory. First download the latest release of QE as a zipped archive:

```
$ wget https://gitlab.com/QEF/q-e/-/archive/qe-6.4-rc/q-e-qe-6.4-rc.tar.gz
```

Then unpack and remove the zipped archive:

```
$ tar -xzvf q-e-qe-6.4-rc.tar.gz; rm q-e-qe-6.4-rc.tar.gz
```

QE is now unpacked. It is useful to look inside the directory:

```
$ cd q-e-qe-6.4-rc; l
```

Step 2: Configure QE

To use the program **pw.x** we need to compile the Fortran source into an executable. This operation is performed by the script Makefile. Makefile in turn needs to know where to look for

the compilers and numerical libraries. This information is determined by the program configure. Therefore, we issue:

```
$. /configure ; make pw
```

At the end of the compilation we should find the newly-created executable **pw.x** inside the directory bin:

```
$ ls bin
```