XCONFIGURE

XCONFIGURE is a collection of configure wrapper scripts for various HPC applications. The purpose of the scripts is to configure the application in question to make use of Intel's software development tools (Intel Compiler, Intel MPI, Intel MKL). This may sounds cumbersome, but it actually helps to rely on a "build recipe", which is known to expose the highest performance or to reliably complete the build process.

Each application (or library) is hosted in a separate subdirectory. In order to configure (and ultimately build) an application, one may clone or download the entire collection.

```
git clone https://github.com/hfp/xconfigure.git
```

Alternatively, one can rely on a single script which then downloads a specific wrapper into the current working directory (of the desired application).

```
wget https://github.com/hfp/xconfigure/raw/master/configure-get.sh
./configure-get.sh qe hsw
```

To configure an application, please follow into one of the aforementioned subfolders and read the build recipe of this application e.g., **qe** in case of Quantum Espresso.

Eigenvalue SoLvers for Petaflop-Applications (ELPA)

Download and unpack ELPA, and make the configure wrapper scripts available in ELPA's root folder.

```
wget http://elpa.mpcdf.mpg.de/html/Releases/2016.05.004/elpa-2016.05.004.tar.gz
tar xvf elpa-2016.05.004.tar.gz
cd elpa-2016.05.004
```

Please make the Intel Compiler available on the command line. This actually depends on the environment. For instance, many HPC centers rely on `module load`.

```
source /opt/intel/compilers_and_libraries_2017.0.098/linux/bin/compilervars.sh intel64
```

For example, to configure and make for an Intel Xeon E5v4 processor (formerly codenamed Haswell):

```
./configure-elpa-hsw-omp.sh
make -j ; make install
```

For a further reference, one may have a look at
https://software.intel.com/en-us/articles/quantum-espresso-for-the-intel-xeon-phi-processor.

Quantum Espresso (QE)

Download and unpack Quantum Espresso, and make the configure wrapper scripts available in QE's root folder. However, before one needs to complete the ELPA build recipe!

```
wget http://www.qe-forge.org/gf/download/frsrelease/224/1044/qe-6.0.tar.gz
tar xvf qe-6.0.tar.gz
cd qe-6.0
```

Please make the Intel Compiler available on the command line. This actually depends on the environment. For instance, many HPC centers rely on `module load`.

```
source /opt/intel/compilers_and_libraries_2017.0.098/linux/bin/compilervars.sh intel64
```

For example, configure for an Intel Xeon E5v4 processor (formerly codenamed Haswell), and build the desired application(s) e.g., "pw", "cp", or "all".

```
./configure-qe-hsw-omp.sh
make pw -j
```

For a further reference, one may have a look at
https://software.intel.com/en-us/articles/quantum-espresso-for-the-intel-xeon-phi-processor.