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 sound 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
chmod +x 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.

CP2K

The build and run instructions for CP2K using Intel Tools are exercised at
https://github.com/hfp/libxsmm/tree/master/documentation/cp2k.md (pdf).

Please note, it is beneficial to rely on ELPA, LIBINT, and LIBXC.

Eigenvalue SoLvers for Petaflop-Applications (ELPA)

Build Instructions

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
wget https://github.com/hfp/xconfigure/raw/master/configure-get.sh
chmod +x configure-get.sh
./configure-get.sh elpa
```

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 "Broadwell"):

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

References

https://software.intel.com/en-us/articles/quantum-espresso-for-the-intel-xeon-phi-processor

LIBINT

Build Instructions

TBD

References

TBD

LIBXC

Build Instructions

TBD

References

TBD

LIBXSMM

LIBXSMM is a library targeting Intel Architecture (x86) for small, dense or sparse matrix multiplications, and small convolutions. The build instructions can be found at https://github.com/hfp/libxsmm (pdf).

Quantum Espresso (QE)

Build Instructions

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

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 "Broadwell"), and build the desired application(s) e.g., "pw", "cp", or "all".

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

Run Instructions

TBD

References

https://software.intel.com/en-us/articles/quantum-espresso-for-the-intel-xeon-phi-processor