

# [Q-e-developers] ELPA for QE, instructions to build latest version working after r13250

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Hello everybody,

in QE v6.0, we support ELPA version 2016.05.003 [1]. This version of ELPA has the ability to deliver better performance than plain ScaLAPACK but it has also have a different API that the former versions or the early legacy ELPA we ship as part of the QE distribution.

A new released version of ELPA is available publicly which support KNL and GPU (2016.11.001\_pre [2]). However the API have changed again. We raised this issue to the ELPA developers but until they fix and stabilize the library API, some changes need to be made in the source code to support 2016.11.001\_pre.

Here a short guide how to compile ELPA first and QE with ELPA.

## # Prerequisites

You need ScaLAPACK (and so, BLACS) installed correctly in your system. You can find them in the Intel MKL / Intel MPI bundles or you have to download source codes and install by yourself. My suggestion is to use Intel MKL.

## # Download and compile ELPA

ELPA 2016.11.001\_pre is available here = [https://elpa.mpcdf.mpg.de/html/Releases/2016.11.001\\_pre/elpa-2016.11.001\\_pre.tar.gz](https://elpa.mpcdf.mpg.de/html/Releases/2016.11.001_pre/elpa-2016.11.001_pre.tar.gz)

To compile simply run the configure and then "make". You need to check that \$MKLR00T points where the MKL are installed. You can chose to enable OpenMP (--enable-openmp) or not (--disable-openmp). \$SCALAPACK\_FCFLAGS and \$SCALAPACK\_LDFLAGS will have to change accordingly in order to link the correct math libraries.

```
./configure --enable-openmp --prefix=$PREFIX SCALAPACK_LDFLAGS="-L${MKLR00T}/lib/intel64
-lmkl_scalapack_lp64 -lmkl_blacs_intelmpi_lp64 -lmkl_intel_lp64 -lmkl_core
-lmkl_intel_thread -lpthread -lm" SCALAPACK_FCFLAGS="-L${MKLR00T}/include"
```

\$PREFIX is where you want to deploy the library (e.g. a central folder in a cluster or your home directory).

# Export ELPA environment variables:

In ELPA the way "make install" operates does create an additional directory under "include/" which confuses current autoconf. To avoid failing over and over, we made the configure relying on the user who has to specify where the right headers are located. Assuming \$PREFIX points to the directory where you installed ELPA by doing "make install", here how to export some environment variables that we will use later with QE

```
export ELPA_HOME=$PREFIX
```

```
X=`ls -l $ELPA_HOME/lib/pkgconfig/`  
export ELPA_VERSION=`echo "${X%.*}"`
```

```
export ELPA_LIBS=$ELPA_HOME/lib  
export ELPA_C_INCLUDE=$ELPA_HOME/include/$ELPA_VERSION/elpa  
export ELPA_FORTRAN_INCLUDE=$ELPA_HOME/include/$ELPA_VERSION/modules
```

```
export PATH=$ELPA_HOME/bin:$PATH  
export LD_LIBRARY_PATH=$ELPA_LIB:$LD_LIBRARY_PATH
```

# Compile QE with ELPA pre-compiled (this works only for r13250)

Example with MPI and OpenMP both enabled, ELPA linked statically:

```
./configure --enable-openmp --enable-parallel --with-scalapack=intel --with-elpa-lib=$ELPA_LIBS/libelpa_openmp.a --with-elpa-include=$ELPA_FORTRAN_INCLUDE
```

My personal hope is to see ELPA API fixed (or stabilized) by the time a new QE release is created. In the meanwhile, we will continue to monitor ELPA changes. Ideally, we do not want to support too many versions that have different or broken API.

HTH

Cheers

- [1] <https://elpa.mpcdf.mpg.de/html/Releases/2016.05.003/>
- [2] <https://elpa.mpcdf.mpg.de/html/Releases/2016.11.001.pre/>

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