Introduction to QUANTUM ESPRESSO for would-be developers

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Developers' Resources

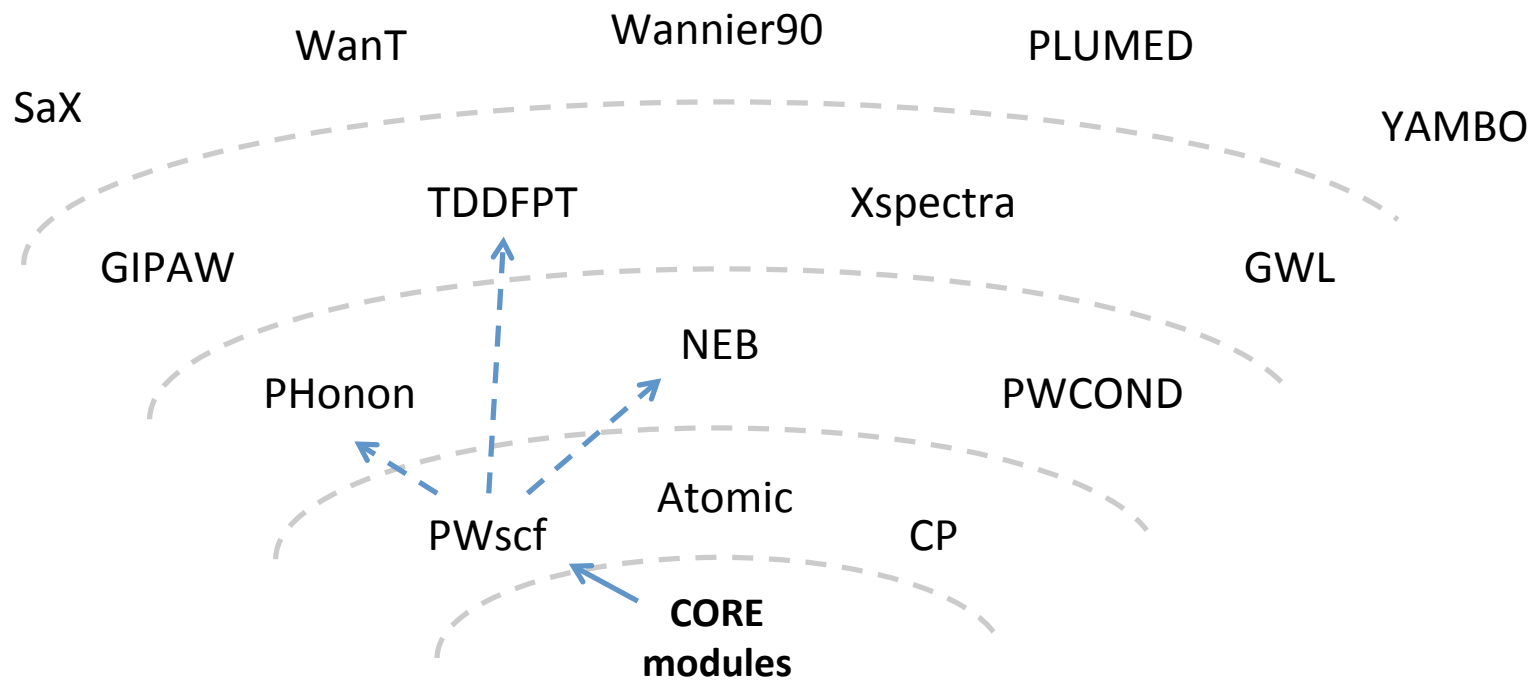
When everything else fails, read the manual!

There isn't a real QUANTUM ESPRESSO manual, but there are some useful resources for developers:

- the pseudo-manual `Doc/developers-man.pdf`, plus other files in `Doc/`, `install/`, `include/`;
- scattered documentation in source files;
- `www.quantum-espresso.org`, *Resources* menu, under *Developers' Resources*
- the `q-e` project on `qe-forge.org`, and in particular the bug tracker, forum, mailing list archives, web-svn interface.

The QUANTUM ESPRESSO ecosystem (zoo?)

Quantum ESPRESSO package portfolio



QUANTUM ESPRESSO FOUNDATION

(the above slide courtesy of Filippo Spiga)

Core QUANTUM ESPRESSO distribution

In the following I will refer to the *core* distribution, including

- scripts, installation tools, libraries, common source files;
- basic packages
  - `PWscf`: self-consistent calculations, structural optimization, molecular dynamics on the ground state;
  - `CP`: Car-Parrinello molecular dynamics;
  - `PostProc`: data analysis and plotting (requires `PWscf`)

All of the above is stored into a single ('main') SVN repository.
Some libraries are however downloaded on demand from the web.

Most of what will be said is valid also for *additional* packages.

More QUANTUM ESPRESSO distribution

Additional packages that can be downloaded and installed on demand:

- `atomic`: pseudopotential generation
- `PHonon`: Density-Functional Perturbation Theory
- `NEB`: reaction pathways and energy barriers
- `PWCOND`: ballistic conductance
- `XSPECTRA`: calculation of X-Ray spectra
- `TDDFPT`: Time-dependent DFPT (requires `PHonon`)

All these *require that the core distribution is already installed*.
Stored in the main SVN repository along with the core distribution.

Additional QUANTUM ESPRESSO pieces

More packages that can be downloaded and installed on demand:

- `GIPAW`: calculation of NMR coefficients and chemical shifts.
  Stored in separate SVN repository that can be downloaded into the main SVN repository

- `EPW`: electron-phonon (under development, requires `PHonon`).
  SVN: as above

A further package that depends upon the core QUANTUM ESPRESSO distribution (must be separately downloaded and installed):

- `GWL`: GW calculations using Lanczos chains.

Directory structure of QUANTUM ESPRESSO

Common files and directories in the `espresso/` directory:

- `install/`
- `include/`
- `archive/`
- `dev-tools/`
- `pseudo/`
- `Doc/`
- `clib/`
- `Modules/`
- `PW/`
- `CPV/`
- `configure`
- `make.sys`
- `Makefile`
- `License`
- `README`
- `environment_variables`
- `flib/`
- `upftools/`
- `PP/`

`PW/`, `PP/`, `CPV/` are specific for the respective packages: `PWscf`, `PostProc`, `CP`. The rest is the common part.

Common Files and Directories

Apart from `License` and `README` whose meaning is obvious, the other files and directories are related to

- *Installation* (i.e. compilation and linking):
  `install/`, `dev-tools/`, `archive/`, `configure`, `make.sys`
- *Testing* (running tests and examples):
  `pseudo/`, `environment_variables`
- *General documentation* (not package-specific): `Doc/`
- *C and Fortran Libraries, modules* (F95): `clib/`, `flib/`, `Modules/`

Files and Directories in a Packages

Typical subdirectories of a directory containing a package (e.g. `PW/`):

```
Makefile
examples/
tests/
Doc/
src/
```

Note that:

- `tests/` contains automated post-installation tests (only in `PW/` and `CPV/`) while `examples/` are not suitable for automated checks
- other packages may have a slightly different structure (in particular, `PHonon` has three directories for sources and none is called `src/`)

Compilation and linking

QUANTUM ESPRESSO requires a number of machine-dependent pre-processing, compilation, linking options to be set; plus a number of libraries to be available. Packages can be downloaded, compiled and linked on demand. This is achieved using `configure` and `make` utilities. Files related to compilation and linking:

`install/`: documentation and utilities for compilation and linking

`configure`: wrapper for `install/configure` script

`make.sys`: file produced by running `configure`, used by `Makefile`, contains machine-specific compilation and linking options

`Makefile`: contains dependencies and targets used by command `make`.

`include/`: files to be included into sources, to be pre-processed

Compilation and linking (2)

"`./configure` *options*" runs `install/configure`, produces file `make.sys`. Its behavior can be changed by modifying file `install/configure.ac` and running (in `install/`) command `autoconf`. This produces a new version of `install/configure`.

"`make` *target*" checks for dependencies, recursively goes into subdirectories executing `make` again. The behavior of `make` is thus determined by many `Makefile`'s in the various directories. The most important files are `Makefile`'s in the directories containing sources, e.g. `Modules/Makefile`, `PW/src/Makefile`.

Dependencies of Fortran files are contained in `make.depend` files in each source directory. These files *must be updated* if you change the sources, using script `install/makedeps.sh` or running "`make depend`"

The `make.sys` file

Produced by `configure`, contains all system-specific information on

- C and Fortran compilers name, pre-processing and compilation options
- whether the Fortran compiler performs C-style preprocessing or not
- whether compiling for parallel or serial execution
- available optimized mathematical libraries, libraries to be downloaded
- Miscellanous stuff

Written for usage into `Makefile`'s, using the corresponding syntax.

The best documentation for the `make.sys` file is the file itself.

Makefile

The top-level Makefile contains the instructions to download, unpack, compile and link what is required. Sample contents:

```
include make.sys
```

Contains machine- and QUANTUM ESPRESSO*-specific definitions*

```
default :
   @echo 'to install, type at the shell prompt:'
   ...
```

If no target specified, ask for one, giving a list of possibilities

```
pw : bindir mods liblapack libblas libs libiotk libenviron
   if test -d PW ; then \
   ( cd PW ; if test "$(MAKE)" = "" ; then make $(MFLAGS) T
     else $(MAKE) $(MFLAGS) TLDEPS= all ; fi ) ; fi
```

Target `pw`*: first check the list of dependencies* `bindir mods ...` *etc., do what is needed; then go into* `PW/` *and give command* `make all`

```
neb : bindir mods libs pw
    cd install ; $(MAKE) $(MFLAGS) -f plugins_makefile $@
```

Target `neb`*: do all of the above, then go into directory* `install/` *where* `make neb` *using* `plugins_makefile` *as Makefile will check if NEB is there, download from the network if not, compile and link it*

```
libblas : touch-dummy
     cd install ; $(MAKE) $(MFLAGS) -f extlibs_makefile $@
```

Target `libblas`*: this is an external library, that may or may not be needed, depending upon what is written in* `make.sys`*. If needed, go into directory* `install/` *where* `make libblas` *using* `extlibs_makefile` *as Makefile will check if BLAS are there, download from the network if not, compile and build the library*

PW/Makefile

Second-level Makefile contains only targets related to a given subdirectory or package. Sample contents:

```
default : all
all: pw pwtools
pw:
    if test -d src ; then \
    ( cd src ; if test "$(MAKE)" = "" ; then make $(MFLAGS)
      else $(MAKE) $(MFLAGS) ; fi ) ; fi ; \
...
```

Target `pw`*: go into* `src/` *if it exists, and (apart from* `make` *wizardry you don't want to know about) give command* `make pw`*. Other targets are quite similar: go into a subdirectory, e.g.* `Doc/` *and '*`make` *something', e.g.* `make clean`*.*

PW/src/Makefile

The most important and most complex Makefile is the one in the source directory. It is also the one you need to modify if you add something.

```
include ../../make.sys
```

Contains machine- and QUANTUM ESPRESSO*-specific definitions*

```
MODFLAGS= $(MOD_FLAG)../../iotk/src
          $(MOD_FLAG)../../Modules $(MOD_FLAG).
```

Location of needed modules; `MOD_FLAG` *is defined in* `make.sys`

```
PWOBJS = \
pwscf.o
```

Object file containing main program (this is actually redundant)

```
PWLIBS = \
a2fmod.o \
...
wannier_enrg.o
```

List of objects - add here new objects, or delete from this list. Do not forget the backslash! It ensure continuation of the line

```
QEMODS=../../Modules/libqemod.a
```

Objects from `Modules/` *are available from the above archive. The directory where F95 modules are must also be specified to the compiler!*

```
TLDEPS=bindir mods libs liblapack libblas libenviron
```

TLDEPS=Top-Level DEPendencieS: a machinery to ensure proper compilation with correct dependencies also if compiling from inside a package directory and not from top level

```
LIBOBJS = ../../flib/ptools.a ../../flib/flib.a
          ../../clib/clib.a   ../../iotk/src/libiotk.a
```

All needed QE-specific libraries

```
all : tldeps pw.x generate_vdW_kernel_table.x
```

Targets that will be build - add here new executables

```
pw.x : $(PWOBJS) libpw.a $(LIBOBJS) $(QEMODS)
     $(LD) $(LDFLAGS) -o $@ \
     $(PWOBJS) libpw.a $(QEMODS) $(LIBOBJS) $(LIBS)
   - ( cd ../../bin; ln -fs ../PW/src/$@ . )
```

Target `pw.x` *- produces executable with the same name. It also produces a link to the executable in* `espresso/bin/`*. Do not forget tabulators even if you do not see them! All variables (introduced by $) are either defined locally in* `Makefile` *or imported from* `make.sys`

```
libpw.a : $(PWLIBS)
        $(AR) $(ARFLAGS) $@ $?
        $(RANLIB) $@
```

This builds the library libpw.a - again, do not forget tabulators

```
tldeps:
       test -n "$(TLDEPS)" && ( cd ../.. ;
       $(MAKE) $(MFLAGS) $(TLDEPS) || exit 1) || :
```

second part of the TLDEPS machinery

```
clean :
    - /bin/rm -f *.x *.o *.a *~ *.F90 *.d *.mod *.i *.L
```

There should always be a "clean" target, removing all compiled (.o) or preprocessed (*.F90) stuff - compiled F95 modules may have different filenames: the four last items cover most cases*

`include make.depend`

Contains dependencies of objects upon other objects. Sample content of file `make.depend` *(can be produced by* `install/makedep.sh`*):*

```
a2fmod.o : ../../Modules/io_global.o
a2fmod.o : ../../Modules/ions_base.o
a2fmod.o : ../../Modules/kind.o
a2fmod.o : pwcom.o
a2fmod.o : start_k.o
a2fmod.o : symm_base.o
```

tells us that the listed objects must have been compiled prior to compilation of a2fmod.o - `make` *will take care of this.*

BEWARE: the Makefile system is in a stable but delicate equilibrium, resulting from many years if experiments on many different machines. Handle with care: what works for you may break other cases.

Directories containing sources

- `clib/`: a few routines written in C: FFTW, system calls. May include `*.h` files in `include/`, notably `c_defs.h`, using the CPP syntax `#include 'c_defs.h'`.

- `flib/`: Spherical Bessel functions, Spherical Harmonics, exch-corr functionals, basic and utility routines written in Fortran-95

- `Modules/`: basic Fortran-95 modules used by all packages

- `PW/src/`: package-specific Fortran-95 main and subroutines

Order of compilation: external libraries (e.g. BLAS, LAPACK) first; then `clib/`, `Modules/`, `flib/`, `PW/src/`

Note: distinction between `flib/` and `Modules/` is by now obsolete

Preprocessing

Fortran-95 source code contains pre-processing option with CPP syntax. Most F95 compilers understand pre-processing options `-D ...` or some similar form. Pre-processing is useful to

- account for machine dependency in a unified source tree
- distinguish between parallel and serial execution when they follow different paths (i.e. there is a substantial difference between serial execution and parallel execution on a single processor)
- introduce experimental or special-purpose stuff

Use with care and *only when needed*. See file `include/defs.README` for a list of pre-processing options. Please *keep that list updated*.

Note: `include/f_defs.h` is obsolete and must not be used any longer.

Examples of preprocessing (1)

`flib/flush_unit.f90`:

```
#if defined(__XLF) || defined(__ABSOFT)
   #define flush flush_
#endif
[...]
  !
  IF ( opnd ) CALL flush( unit_tobeflushed )
  !
```

in XLF and ABSOFT compilers,the system routine `flush`*, emptying output buffers, needs an underscore at the end.* `__XLF` *or* `__ABSOFT` *are defined in* `make.sys` *as pre-processing variables at compile time.*

Examples of preprocessing (2)

`flib/sph_bes.f90`:

```
#if defined (__MASS)
      qr = q * r
      call vcos( cos_qr, qr, msh)
      jl = cos_qr / qr
#else
      jl (:) = cos (q * r (:) ) / (q * r (:) )
#endif
```

if `__MASS` *is defined, use the IBM mathematical fast routines MASS.* `configure` *finds out whether these routines actually exists for the machine you are compiling on.*

Modules/environment.f90:

```
#ifdef __MPI
    CALL parallel_info ( )
#else
    CALL serial_info()
#endif
[...]
  SUBROUTINE parallel_info ( )
#if defined(__OPENMP)
    INTEGER, EXTERNAL :: omp_get_max_threads
#endif
```

if `__MPI` *is defined, the code is compiled for parallel execution. A different routine is called wrt the serial case. __OPENMP accounts for OpenMP parallelization. Note that __PARA and __MPI are used as synonims, but the former shouldn't be used any longer.*