QUANTUMESPRESSO

A GENERAL OVERVIEW BY GABRIELE MOGNI

WHAT IS QUANTUM ESPRESSO?

- Quantum ESPRESSO is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale.
  It is based on density-functional theory, plane waves, and pseudopotentials.
- Quantum ESPRESSO has evolved into a distribution of independent and inter-operable codes in the spirit of an open-source project. The Quantum ESPRESSO distribution consists of a "historical" core set of components, and a set of plug-ins that perform more advanced tasks, plus a number of third-party packages designed to be inter-operable with the core components. Researchers active in the field of electronic-structure calculations are encouraged to participate in the project by contributing their own codes or by implementing their own ideas into existing codes.

WHAT CAN QE DO?

- Ground-state calculations.
- Structural Optimization.
- Transition states and minimum energy paths.
- Ab-initio molecular dynamics.
- Response properties (DFPT).
- Spectroscopic properties.
- Quantum Transport.
- Platforms.

GROUND STATE CALCULATIONS

- Self-consistent total energies, forces, stresses;
- Kohn-Sham orbitals;
- Separable norm-conserving and ultrasoft (Vanderbilt) pseudo-potentials, PAW (Projector Augmented Waves);
- Several exchange-correlation functionals: from LDA to generalized-gradient corrections (PW91, PBE, B88-P86, BLYP) to meta-GGA, exact exchange (HF) and hybrid functionals (PBE0, B3LYP, HSE);
- VdW corrections (DFT-D) or nonlocal VdW functionals (vdw-DF);
- Hubbard U (DFT+U);
- Berry's phase polarization;
- Spin-orbit coupling and noncollinear magnetism.

STRUCTURAL OPTIMIZATION

- GDIIS with quasi-Newton BFGS preconditioning;
- Damped dynamics.

TRANSITION STATES AND MINIMUM ENERGY PATHS

- Nudged Elastic Band method;
- Meta-Dynamics, using the PLUMED plug-in.

AB-INITIO MOLECULAR DYNAMICS

- Car-Parrinello Molecular Dynamics (CP package);
- Born-Oppenheimer Molecular Dynamics (PWscf package).

RESPONSE PROPERTIES (DFPT)

- Phonon frequencies and eigenvectors at any wavevector;
- Full phonon dispersions; inter-atomic force constants in real space;
- Translational and rotational acoustic sum rules;
- Effective charges and dielectric tensors;
- Electron-phonon interactions;
- Third-order anharmonic phonon lifetimes, using the D3Q package;
- Infrared and (non-resonant) Raman cross-sections;
- EPR and NMR chemical shifts, using the QE-GIPAW package.

SPECTROSCOPIC PROPERTIES

- K-, L_1 and $L_{2,3}$-edge X-ray Absorption Spectra (XSpectra package);
- Time-Dependent Density Functional Perturbation Theory (TurboTDDFT package);
- Electronic excitations with Many-Body Perturbation Theory, using the YAMBO package;
- Electronic excitations with Many-Body Perturbation Theory (GWL package).

QUANTUM TRANSPORT

- Ballistic Transport (PWCOND package);
- Coherent Transport from Maximally Localized Wannier Functions, using the WanT code;
- Maximally-localized Wannier functions and transport properties, using the WANNIER90 code.

PLATFORMS

- Runs on almost every conceivable current architecture (really! also cell phones and playstations): from large parallel machines (IBM SP and BlueGene, Cray XT, Altix, Nec SX) to workstations (HP, IBM, SUN, Intel, AMD) and single PCs running Linux, Windows, Mac OS-X, including clusters of 32-bit or 64-bit Intel or AMD processors with various connectivity (gigabit ethernet, myrinet, infiniband…). Fully exploits math libraries such as MKL for Intel CPUs, ACML for AMD CPUs, ESSL for IBM machines.
  GPU-enabled version available via the QE-GPU add-on package.

The QUANTUM ESPRESSO codes work on many different types of Unix machines, including parallel machines using both OpenMP and MPI (Message Passing Interface) and GPU-accelerated machines. QUANTUM ESPRESSO also runs on Mac OS X and MS-Windows machines: see section 2.2.

Further documentation, beyond what is provided in this guide, can be found in:

- the `Doc/` directory of the QUANTUM ESPRESSO distribution;
- the QUANTUM ESPRESSO web site `www.quantum-espresso.org`;
- the archives of the mailing list: See section 1.2, "Contacts", for more info.

GENERAL OVERVIEW

- The full Quantum ESPRESSO distribution contains the following core packages for the calculation of electronic-structure properties within Density-Functional Theory (DFT), using a Plane-Wave basis set and pseudopotentials:

- PWscf (PW) : Plane-Wave Self-Consistent Field,
- CP (CPV): Car-Parrinello Molecular Dynamics.

- It also includes the following more specialized packages:

- PWneb (NEB) : energy barriers and reaction pathways through the Nudged Elastic Band method,
- PHonon : phonons with Density-Functional Perturbation Theory,
- PostProc (PP) : various utilities for data postprocessing,
- PWcond : ballistic conductance,
- XSPECTRA : K-edge X-ray adsorption spectra,
- GIPAW (Gauge-Independent Projector Augmented Waves): NMR chemical shifts and EPR g-tensor.
- TDDFPT : calculations of spectra using Time-Dependent Density-Functional Perturbation Theory.

- The following auxiliary codes are included as well:

- PWgui : a Graphical User Interface, producing input data files for PWscf,
- atomic : a program for atomic calculations and generation of pseudopotentials.
- QHA : utilities for the calculation of projected density of states (PDOS) and of the free energy in the Quasi-Harmonic Approximation (to be used in conjunction with PHonon).
- PlotPhon : phonon dispersion plotting utility (to be used in conjunction with PHonon).

- Several additional packages that exploit data produced by Quantum ESPRESSO or patch some Quantum ESPRESSO routines can be installed as plug-ins:

- WANNIER90 : maximally localized Wannier functions.
- WanT: quantum transport properties with Wannier functions.
- YAMBO: electronic excitations within Many-Body Perturbation Theory: GW and Bethe-Salpeter equation.
- PLUMED: calculation of free-energy surface through metadynamics.
- GIPAW (Gauge-Independent Projector Augmented Waves): NMR chemical shifts and EPR g-tensor.
- GWL: electronic excitations within GW Approximation.
- WEST: Many-body perturbation corrections for standard DFT.

PWSCF (PW), PLANE-WAVE SELF-CONSISTENT FIELD

1.1 What can PWscf do

PWscf performs many different kinds of self-consistent calculations of electronic-structure properties within Density-Functional Theory (DFT), using a Plane-Wave (PW) basis set and pseudopotentials (PP). In particular:

- ground-state energy and one-electron (Kohn-Sham) orbitals, atomic forces, stresses;
- structural optimization, also with variable cell;
- molecular dynamics on the Born-Oppenheimer surface, also with variable cell;
- macroscopic polarization and finite electric fields via the modern theory of polarization (Berry Phases);
- modern theory of orbital magnetization;
- free-energy surface calculation at fixed cell through meta-dynamics, if patched with PLUMED.

PWSCF (PW)

All of the above works for both insulators and metals, in any crystal structure, for many exchange-correlation (XC) functionals (including spin polarization, DFT+U, meta-GGA, non-local and hybrid functionals), for norm-conserving (Hamann-Schluter-Chiang) PPs (NCPPs) in separable form or Ultrasoft (Vanderbilt) PPs (USPPs) or Projector Augmented Waves (PAW) method. Noncollinear magnetism and spin-orbit interactions are also implemented. An implementation of finite electric fields with a sawtooth potential in a supercell is also available.

2 Compilation

`PWscf` is included in the core QUANTUM ESPRESSO distribution. Instruction on how to install it can be found in the general documentation (User's Guide) for QUANTUM ESPRESSO.

Typing `make pw` from the main QUANTUM ESPRESSO directory or `make` from the `PW/` subdirectory produces the `pw.x` executable in `PW/src` and a link to the `bin/` directory. In addition, several utility programs, and related links in `bin/`, are produced in `PW/tools`:

- `PW/tools/dist.x` reads input data for `PWscf`, calculates distances and angles between atoms in a cell, taking into account periodicity

- `PW/tools/ev.x` fits energy-vs-volume data to an equation of state

- `PW/tools/kpoints.x` produces lists of k-points

- `PW/tools/pwi2xsf.sh`, `pwo2xsf.sh` process respectively input and output files (not data files!) for `pw.x` and `neb.x` (the latter, courtesy of Pietro Bonfà) and produce an XSF-formatted file suitable for plotting with XCrySDen: `http://www.xcrysden.org/`, a powerful crystalline and molecular structure visualization program. BEWARE: the `pwi2xsf.sh` shell script requires the `pwi2xsf.x` executables to be located somewhere in your PATH.

- `PW/tools/bs.awk`, `PW/tools/mv.awk` are scripts that process the output of `pw.x` (not data files!). Usage:

```
awk -f bs.awk < my-pw-file > myfile.bs
awk -f mv.awk < my-pw-file > myfile.mv
```

  The files so produced are suitable for use with `xbs`, a very simple X-windows utility to display molecules, available at:
  `http://www.ccl.net/cca/software/X-WINDOW/xbsa/README.shtml`

- `PW/tools/cif2qe.sh`: script converting from CIF (Crystallographic Information File) to a format suitable for QUANTUM ESPRESSO. Courtesy of Carlo Nervi (Univ. Torino, Italy).

3 Using PWscf

Input files for `pw.x` may be either written by hand or produced via the `PWgui` graphical interface by Anton Kokalj, included in the QUANTUM ESPRESSO distribution. See `PWgui-x.y.z/INSTALL` (where x.y.z is the version number) for more info on `PWgui`, or `GUI/README` if you are using SVN sources.

3.1 Input data

Input data is organized as several namelists, followed by other fields ("cards") introduced by keywords. The namelists are

&CONTROL:	general variables controlling the run
&SYSTEM:	structural information on the system under investigation
&ELECTRONS:	electronic variables: self-consistency, smearing
&IONS (optional):	ionic variables: relaxation, dynamics
&CELL (optional):	variable-cell optimization or dynamics

Optional namelist may be omitted if the calculation to be performed does not require them. This depends on the value of variable `calculation` in namelist &CONTROL. Most variables in namelists have default values. Only the following variables in &SYSTEM must always be specified:

`ibrav`	(integer)	Bravais-lattice index
`celldm`	(real, dimension 6)	crystallographic constants
`nat`	(integer)	number of atoms in the unit cell
`ntyp`	(integer)	number of types of atoms in the unit cell
`ecutwfc`	(real)	kinetic energy cutoff (Ry) for wavefunctions.

After the namelists, you have several fields ("cards") introduced by keywords with self-explanatory names:

ATOMIC_SPECIES
ATOMIC_POSITIONS
K_POINTS
CELL_PARAMETERS (optional)
OCCUPATIONS (optional)

Note about k points: The k-point grid can be either automatically generated or manually provided as a list of k-points and a weight in the Irreducible Brillouin Zone only of the Bravais lattice of the crystal. The code will generate (unless instructed not to do so: see variable `nosym`) all required k-points and weights if the symmetry of the system is lower than the symmetry of the Bravais lattice. The automatic generation of k-points follows the convention of Monkhorst and Pack.

For metallic systems, you have to specify how metallicity is treated in variable `occupations`. If you choose `occupations='smearing'`, you have to specify the smearing type `smearing` and the smearing width `degauss`. Spin-polarized systems are as a rule treated as metallic system,

Example: fcc-Cu

```
 &control
    calculation='scf'
    restart_mode='from_scratch',
    pseudo_dir = '/home/seitsonen/usr/espresso/PP_LIBRARY/',
    wfcdir='/tmp/'
    prefix='fcc-Cu'
    tstress = .true.
    tprnfor = .true.
 /
 &system
    ibrav = 2, a = 4.00, b = 4.00, c = 4.00,
    nat= 1, ntyp= 1,
    nbnd = 9
    ecutwfc = 140
!    ecutrho = 0
    occupations='smearing', smearing='fermi-dirac', degauss=.00367490107593722133
 /
 &electrons
    diagonalization='david'
    conv_thr = 1.0e-9
    mixing_beta = 0.8
 /
ATOMIC_SPECIES
 Cu  63.5500 Cu_pbe-20071125.UPF
ATOMIC_POSITIONS angstrom
 Cu  0.0 0.0 0.0
K_POINTS (automatic)
 16 16 16 0 0 0
```

TYPES OF ELECTRONIC STRUCTURE CALCULATIONS

- Single-point (fixed-ion) SCF calculation
- Band structure calculation
- Noncollinear magnetization, spin-orbit interactions
- DFT+U
- Dispersion Interactions (DFT-D)
- Hartree-Fock and Hybrid functionals
- Dispersion interaction with non-local functional (vdW-DF)
- Polarization via Berry Phase
- Finite electric fields
- Orbital magnetization

TYPES OF OPTIMIZATION AND DYNAMICS CALCULATIONS

- Structural optimization
- Molecular Dynamics
- Free-energy surface calculations
- Variable-cell optimization
- Variable-cell molecular dynamics

POSTPROC (PP), POST-PROCESSING AND ANALYSIS TOOLS

The main postprocessing code `pp.x` extracts the specified data from the data files produced by `PWscf` (`pw.x` executable) or `CP` (`cp.x` executable); prepares data for plotting by writing them into formats that can be read by several plotting programs.

Quantities that can be read or calculated are:

- charge density
- spin polarization
- various potentials
- local density of states at E_F
- local density of electronic entropy
- STM images
- selected squared wavefunction
- ELF (electron localization function)
- RDG (reduced density gradient)
- integrated local density of states

Various types of plotting (along a line, on a plane, three-dimensional, polar) and output formats (including the popular cube format) can be specified. Moreover data can be saved to an intermediate (formatted) file so that more data set can be summed or subracted in a later run. The output files can be directly read by the free plotting system Gnuplot (1D or 2D plots), or by code `plotrho.x` that comes with `PostProc` and produces PostScript 2D plots, or by advanced plotting software XCrySDen and gOpenMol (3D plots).

USER TOOLS

- Input data can be prepared using the graphical user interface PWGui, by Anton Kokalj
- An alternative graphical user interface running on WIndows: Burai, by Satomichi Nishihara
- Visualization of the results can be obtained using XCrySDen
- An experimental web-based interface is available at NERSC: see the presentation video, contact the authors if interested in trying it
- Other visualization software that can produce input data or read output data for Quantum ESPRESSO:
- GDIS
- J-ICE (on-line converter available at this link)
- VMD
- gOpenMol
- VESTA.

USER TOOLS

•Quantum ESPRESSO *plug-ins* (i.e. software that add functionalities by modifying QE code):
•PLUMED: Meta-Dynamics
•Environ: self-consistent continuum solvation model
•External software using Quantum ESPRESSO code:
•thermo_pw: Elastic constants, Vibrational properties in the Quasi-Harmonic Approximation
•QE-GIPAW: EPR and NMR chemical shifts
•WEST: Electronic excitations with Many-Body Perturbation Theory
•GWL: Electronic excitations with Many-Body Perturbation Theory
•EPW: Calculation of electron-phonon interactions coefficients

USER TOOLS

•External software that can either use QE as a quantum engine, or use QE output data for further processing
•AiiDA: Automated Interactive Infrastructure and Database for Computational Science
•YAMBO: Electronic excitations with Many-Body Perturbation Theory
•WanT: Coherent Transport from Maximally Localized Wannier Functions
•WANNIER90: Maximally-localized Wannier functions and transport properties
•BerkeleyGW: Many-Body Perturbation Theory
•QMCPACK: Quantum Monte Carlo calculations
•ElaStic: Elastic Constants
•XtalOpt: Evolutionary/Genetic Algorithm (no longer maintained)
•USPEX: Evolutionary/Genetic Algorithm
•PHON: Phonon calculation using the Frozen-Phonon approach
•phononpy: Phonon calculation using the Frozen-Phonon approach
•CALYPSO: Crystal structure prediction via Particle Swarm Optimization
•NanoTCAD ViDES: Simulation of nanostructured devices
•BoltzTraP: Calculation of transport properties
•AMULET: Dynamical Mean Field Theory calculations
•PYXAID: non-adiabatic Molecular Dynamics
•Other QE resources found in external sites:
•Virtual NanoLab (VNL) graphical user interface, a free product by QuantumWise
•NanoHub