The QUANTUM ESPRESSO distribution

The IOM-DEMOCRITOS center of Italian CNR is dedicated to atomistic simulations of materials, with a strong emphasis on the development of high-quality scientific software

QUANTUM ESPRESSO is the result of a IOM-DEMOCRITOS initiative, in collaboration with several other institutions (ICTP, CINECA Bologna, EPF Lausanne, Princeton University, Paris VI, IJS Ljubljana,...)

QUANTUM ESPRESSO is an integrated software suite for atomistic simulations based on electronic structure, using density-functional theory (DFT), a plane waves (PW) basis set and pseudopotentials (PP)

QUANTUM ESPRESSO stands for *Quantum opEn-Source Package for Research in Electronic Structure, Simulation, and Optimization*

License

QUANTUM ESPRESSO is distributed under the *GNU (Gnu's Not Unix) General Public License (GPL)*, probably the most common free-software license (e.g.: the Linux Kernel). Basically:

- The source code is available.
- You can do whatever you want with the sources, but if you distribute any derived work, you have to distribute under the GPL the sources of the derived work.

Advantages:

- Everybody – including commercial entities – can contribute.
- Nobody can "steal" the code and give nothing back to the community.

QUANTUM ESPRESSO as a distribution

QUANTUM ESPRESSO is a *distribution* of packages, rather than a single monolithic tightly integrated package. The core distribution contains the two main packages:

- `PWscf`: self-consistent electronic structure, structural optimization, molecular dynamics on the electronic ground state
- `CP`: variable-cell Car-Parrinello molecular dynamics STM maps, etc.)

They share a common installation method, input format, PP format, data output format, large parts of the basic code. Also included:

- `PostProc`: graphical and postprocessing utilities (band structure, density of states, STM maps, ...)

Packages

A set of packages, using routines from the core distribution, can be downloaded and installed on demand:

- `PWGui`: a Graphical User Interface for production of input files
- `PHonon`: linear-response calculations (phonons, dielectric properties)
- `NEB`: reaction pathways and barriers using Nudged Elastic Band
- `atomic`: atomic calculations, pseudopotential generation
- `PWcond`: ballistic conductance
- `XSpectra`: X-ray near-edge adsorption spectra (XANES) shifts
- `TDDFPT`: Time-Dependent Density-Functional Perturbation Theory

Plug-ins

More advanced features, interoperable "external" packages:

- `GIPAW`: Gauge-Independent PAW for EPR and NMR chemical
- `GWL`: GW band structure with ultralocalized Wannier functions
- `PLUMED`: plugin for metadynamics calculations
- `WanT`: Transport using maximally Localised Wannier functions
- `W90`: package for Maximally Localised Wannier functions
- `SaX`: electronic excitations from GW band structure
- `Yambo`: GW band structure, Bethe-Salpeter equations

Organization

Web site: `http://www.quantum-espresso.org`

Newsletter: `pw_users@pwscf.org`, (sparingly) used by developers for announcements about QUANTUM ESPRESSO

Mailing List: `pw_forum@pwscf.org`, for general discussions
(all subscribed users can post)

Developers' portal: `QE-forge`, `http://www.qe-forge.org`
The core distribution and packages is maintained in a single SVN tree.
Available to everyone anytime via anonymous (read-only) access.

Developers' Mailing List: `qe-developers@qe-forge.org` (use this for technical questions or communications to developers)

What can QUANTUM ESPRESSO do?

- $\Gamma-$point and **k**-point calculations, any crystal structure or supercell
- insulators and metals, with various flavors of broadening, or tetrahedra
- norm-conserving PPs in separable form, ultrasoft PPs, PAW
- almost all flavours of LDA and of gradient-corrected exchange-correlation functionals (PW91, PBE, B88-P86, BLYP,...), DFT+U, nonlocal (vdW-DF), hybrid functionals (PBE0, B3LYP), meta-GGA
- spin-polarized, magnetic systems (including noncolinear magnetism and spin-orbit interactions)

on many different hardware and software configurations

Technical characteristics (algorithms)

- use of iterative techniques: the Hamiltonian is stored as operator, not as matrix. All standard PW technicalities: FFT, dual-space, etc., are used. Iterative diagonalization used whenever it is useful.

- fast "double-grid" implementation for ultrasoft PPs: the cutoff for the augmentation part can be larger (the corresponding FFT grid denser in real space) than the cutoff for the smooth part of the charge density.

- Many parallelization levels: on images, on **k**-points, on PW's and FFT grids, on Kohn-Sham states in FFTs, on orthonormalization or subspace diagonalization, for extended scalability up to O(1000) processors.

Technical characteristics (coding)

- written mostly in Fortran-90, with various degrees of sophistication (i.e. use of advanced f90 features) – no dirty tricks, "dusty decks"
- use of standard library routines (lapack, blas, fftw) to achieve portability – Machine-optimized libraries can be used if available
- C-style preprocessing options for machine dependencies (e.g. to select machine-optimized libraries) allow to keep a single source tree
- parallelization via MPI calls, hidden into calls to very few routines – (almost) unified serial and parallel versions. Unless something special is desired, there is no need to know the internals of parallelization in order to write parallel code. OpenMP parallelization is also present.

Easy (or not-so-difficult) installation via the GNU utility `configure`

XML-based data file format

New data format for easy data exchange between different codes:

- a *directory* instead of a single file
- a *formatted* 'head' file contains structural data, computational details, and links to files containing large datasets
- *binary* files for large datasets, one large record per file

Implementation: `iotk` toolkit, written by G. Bussi (ETHZ). Advantages:

- *efficient*: exploits the file system and binary I/O
- *extensible*: based on "fields" introduced by XML syntax
  `<field> ... </field>`
- *easy* to read, write, and understand

Pseudopotential formats

- UPF (Unified Pseudopotential Format):
  - formatted (small amount of data)
  - human-readable (may contain info needed to reproduce the PP)
  - extensible (uses a XML-like syntax)
  - (more) documented (than usual)
  - converters from several some pre-existing formats are available
- Old formats (for compatibility):
  - norm-conserving PP format, one projector per angular momentum
  - norm-conserving and ultrasoft PPs, more than one projector per angular momentum allowed
  - David Vanderbilt's format for ultrasoft PPs

Table of PPs available at `http://www.quantum-espresso.org`

CP package

Car-Parrinello variable-cell molecular dynamics, ultrasoft PPs (Γ only)
Developed by A. Pasquarello (IRRMA, Lausanne), K. Laasonen (Oulu), A. Trave (LLNL), R. Car (Princeton), PG, N. Marzari (MIT); C. Cavazzoni (CINECA), S. Scandolo (ICTP), G. Chiarotti (SISSA), P. Focher, G. Ballabio and others.

- fast treatment ("grid box") of augmentation terms in Ultrasoft PPs
- Various electronic and ionic minimization schemes: damped dynamics, conjugate gradient
- Verlet dynamics with mass preconditioning
- Constrained dynamics
- Nosé thermostat for both electrons and ions, velocity rescaling

CP package, advanced features

- Modified kinetic functional for constant-pressure calculations
- Metallic systems: variable-occupanciy (ensemble) dynamics
- Self-Interaction Correction for systems with one unpaired electron
- Dynamics with Wannier functions under an external electric field
- Finite electric fields with Berry's phase
- MetaGGA functionals
- With `Plumed` plugin: metadynamics (Laio-Parrinello)

PWscf package

Developed by S. Baroni, S. de Gironcoli, A. Dal Corso (SISSA), PG, and others.

- Self-consistent ground-state energy and Kohn-Sham orbitals, forces, structural optimization
- Spin-orbit and noncolinear magnetisation
- Molecular dynamics on the ground-state Born-Oppenheimer surface (no Car-Parrinello dynamics)
- Variable-cell molecular dynamics with modified kinetic functional
- Macroscopic polarization, finite electric fields with Berry's phase
- Advanced functionals: DFT+U, nonlocal, hybrid, metaGGA

PHonon package

- Phonon frequencies and eigenvectors at a generic wave vector
- dielectric tensor, effective charges, IR cross sections
- interatomic force constants in real space
- electron-phonon interaction coefficients for metals
- nonresonant Raman cross sections
- third-order anharmonic phonon lifetimes cross sections

Postprocessing and graphical processing

- Interfaces with XCrySDen and other plotting programs (e.g. VMD)
- Interfaces with other code (e.g. `CASINO`)
- STM maps
- Electron Localization Function (ELF)
- Planar averages
- Density of states (DOS), projected DOS

Pseudopotential generation code

- Norm-Conserving pseudopotentials with either Troullier-Martins or Rabe-Rappe-Kaxiras-Joannopoulos pseudization
- Ultrasoft pseudopotentials (can be build on top of norm-conserving pseudization, but also directly)
- PAW atomic waves (pawsets) can be generated as well

Pseudopotentials can be generated for all exchange-correlation functionals that are implemented in Quantum ESPRESSO

Perspectives and future developments

Work is ongoing in various directions:

- Hybrid functionals in CP with Wannier functions
- Interfaces with genetic/evolutionary algorithm and with QMMM
- Phonons with LDA+U
- Web-based user interface
- ... any other development that people will contribute.

See sec. `People` in the User Guide for the updated list of contributors.

Thanks to all of them!