The Quantum ESPRESSO Software Distribution

The DEMOCRITOS center of Italian INFM 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 DEMOCRITOS initiative, in collaboration with several other institutions (ICTP, CINECA Bologna, EPF Lausanne, Princeton University, MIT)

Quantum ESPRESSO is a distribution of software 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. 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.

The most successful example is probably the Linux Kernel.

Quantum ESPRESSO as a distribution

Quantum ESPRESSO aims at becoming a *distribution* of packages, rather than a single, monolithic, tightly integrated package. Main packages:

- `PWscf`: self-consistent electronic structure, structural relaxation, molecular dynamics
- `CP/FPMD`: variable-cell Car-Parrinello molecular dynamics

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

- `PHonon`: linear-response calculations (phonons, dielectric properties)
- `PostProc`: graphical and postprocessing utilities (density of states, STM, etc.)
- `atomic`: pseudopotential generation code
- `PWGui`: a Graphical User Interface for production of input files

Quantum ESPRESSO as a distribution (2)

More recent or advanced packages:

- `PWcond`: ballistic conductance
- `W90`: Maximally Localised Wannier functions shifts
- `XSpectra`: Calculation of X-ray near-edge adsorption spectra (XANES)
- `GIPAW`: Gauge-Independent PAW method for EPR and NMR chemical

Coming soon:

- `GWW`: GW band structure with ultralocalized Wannier functions
- `TD-DFPT`: Time-Dependent Density-Functional Perturbation Theory

Organization

The distribution is maintained as a single CVS (Concurrent Version System) tree. Available to everyone anytime via anonymous (read-only) access.

- *Web site:* `http://www.quantum-espresso.org`
- *Wiki:* `http://www.quantum-espresso.org/index.php/Main_Page`
  contains the updated documentation
- *Developers' portal:* `http://www.qe-forge.org`
  integrated developer environment, open to external contributions

Mailing lists:

- `pw_users`: used by developers for announcements about Quantum ESPRESSO
- `pw_forum`: for general discussions (all subscribed users can post)

What can Quantum ESPRESSO do?

Quantum ESPRESSO can be used for

- both $\Gamma-$point and **k**-point calculation
- both insulators and metals, with various flavors of broadening, or tetrahedra
- any crystal structure or supercell form
- norm-conserving PP's in separable form, ultrasoft Vanderbilt PP's, PAW
- almost all flavours of LDA and of gradient-corrected exchange-correlation functionals (PW91, PBE, B88-P86, BLYP,...), DFT+U, exact exchange and a few hybrid functionals (PBE0, B3LYP), TPSS 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 PP's: 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.

- Parallelization is performed on both PW's and FFT grids, using a parallel 3D FFT algorithm having good scaling with the number of processors (memory also scales)

- Parallelization on **k**-points and on NEB images is also available by dividing the processors into "pools" and dividing **k**-points/NEB images across pools of processors.

- Further parallelization levels in FFT (task groups), scalable parallel orthonormalization/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, "spaghetti code", "dusty decks"
- use of standard library routines (lapack, blas, fftw) to achieve portability – Machine-optimized libraries can (should!) 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 for all machines
- 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.
- Some degree of OpenMP parallelization

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 tool: `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

Pseudopotentials

PP's must be given in one of the following 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):
  - "Old" norm-conserving PP format, one projector per angular momentum
  - "New" format for both ultrasoft and norm-conserving PP's (more than one projector per angular momentum allowed)
  - David Vanderbilt's format for ultrasoft PP's

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

CP/FPMD package

Car-Parrinello variable-cell molecular dynamics with Ultrasoft PP's (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.

- "Grid Box" for fast treatment of augmentation terms in Ultrasoft PP's
- Various electronic and ionic minimization schemes: damped dynamics, conjugate gradient
- Verlet dynamics with mass preconditioning
- Constrained dynamics
- Temperature control: Nosé thermostat for both electrons and ions, velocity rescaling

CP/FPMD package, advanced features

- Nudged Elastic Band (NEB), Fourier Strings Method schemes for transition paths and energy barriers
- Modified kinetic functional for constant-pressure calculations
- Metallic systems: variable-occupancy 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
- 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
- NEB and Fourier Strings Method schemes for transition paths, energy barriers
- Macroscopic polarization, finite electric fields with Berry's phase
- Exact-exchange calculations, hybrid functionals

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 with other plotting programs (e.g. VMD)
- Interfaces with other codes
- 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
- PAW atomic waves (pawsets) can be generated as well (still at an experimental stage)

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

Perspectives and future developments

New developments and capabilities in the forthcoming new releases:

- Time-Dependent Density-Functional Perturbation Theory
- Better algorithms for electron-phonon interaction coefficients
- More OpenMP parallelization
- Better interoperability with other codes (QMMM!)
- Web-based user interface
- ...

...any other development that people will contribute. See the section `People` in the User Guide for the updated list of contributors. **Thanks to all of them!**