

The Quantum-ESPRESSO Software Distribution

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Democritos and scientific software

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 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*

Why yet another PW-PP-DFT package?

- because it is not another package, but a *merge* of several pre-existing packages, used by many people around the world since a long time
- because it provides access to several techniques whose usefulness has traditionally been hindered by the limited choice of available software: notably
 - *linear response*
 - *ultrasoft PP/PAW*
 - *Car-Parrinello Molecular Dynamics*
 - *parallel computing*
- because a *distribution* that is suitable for easy addition of new packages, developments, extensions, features, is badly needed. Such a goal requires:
 - a *modular* structure, easy to maintain, easily extensible
 - a *collaborative* environment: free/open-source license

On scientific software in physics

Scientific software used in physics tends to belong to one of the following categories:

- *home-brewed*. Typical for small problems: written from scratch – usually in an amateurish way – and left to “bit-rotting” after “publication point” is hit.
- *I-have-my-version*. Typical for bulkier problems (e.g. electronic structure): a package or large code is produced by and distributed to a number of people. Everyone makes its own version, with its own set of changes, additions, subtractions, extensions, incompatibilities.
- *don't-touch-me*. Commercial applications, or applications coming with some form of restrictive license. Often no access to sources, no possibility to do any development, and even if you can, no possibility to re-distribute it. Rather common in chemistry and biology, increasingly common in physics.

The alternative: *free/open-source software*

Free software and GNU license

GNU (Gnu's Not Unix) General Public License (GPL) is 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.

Present status

Main packages in the Quantum-ESPRESSO distribution:

- `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)
- `PP`: graphical and postprocessing utilities (density of states, STM, etc.)
- `atomic`: pseudopotential generation code
- `PWGui`: a Graphical User Interface for production of input files

Present status (2)

More recent or advanced packages:

- PWcond: ballistic conductance
- GIPAW: Gauge-Independent PAW method for EPR and NMR chemical shifts
- W90: Maximally Localised Wannier functions

Already in the CVS version:

- Xspectra: Calculation of X-ray near-edge adsorption spectra (XANES)

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, containing the updated documentation:*
http://www.quantum-espresso.org/index.php/Main_Page

Mailing lists:

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

Coming soon:

- `qe-forge`: an integrated development environment, similar to SourceForge, open to external contributions

What can Quantum-ESPRESSO do?

Quantum-ESPRESSO can be used for

- both Γ -point and \mathbf{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
- 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.

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 (experimental stage)

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
- Electric Field Gradients
- 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:

- Calculation of X-ray spectra (XANES)
- Better algorithms for electron-phonon interaction coefficients
- Time-Dependent Density-Functional Perturbation Theory (TD-DFPT)

...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!**