The Quantum ESPRESSO Software Distribution

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This document introduces to the philosophy of QUANTUM ESPRESSO and describes its main features and capabilities. Further information can be found in

– the documenting papers: J. Phys.: Condens. Matter **21**, 395502 (2009) and J. Phys.: Condens. Matter **29**, 465901 (2017)
– the Web site `www.quantum-espresso.org`
– the users' mailing list `users@lists.quantum-espresso.org`
– the documentation in the `Doc` subdirectories
– the developers' portal `GitLab.com/QEF/q-e`
– the developers' mailing list `developers@lists.quantum-espresso.org`

What is QUANTUM ESPRESSO?

QUANTUM ESPRESSO: *Quantum opEn-Source Package for Research in Electronic Structure, Simulation, and Optimization*, is a *distribution* (an integrated suite) of software for first-principle simulations, i.e., atomistic calculations based on electronic structure, using density-functional theory, a plane-wave basis set, pseudopotentials.

The main goals of QUANTUM ESPRESSO (QE) are

- *innovation* in theoretical methods and numerical algorithms
- *efficiency* on modern computer architectures

A great effort is also devoted to *user friendliness* and to the formation of a *users' and developers' community*

QE exists since 2002, resulting from the merge of pre-existing packages; some core components have been under development for ~ 30 years

License

QE 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 contributors

QE is one of the flagship codes of H2020 project MaX – *Materials at the Exascale*, receives contributions from many individuals and partner institutions in Europe and worldwide. Who "owns" QE ... ?

... the QE Foundation (`foundation.quantum-espresso.org`): a non–profit ("limited by guarantee") company, based in London, that

- coordinates and supports research, education, and outreach within the QE community
- owns the trademarks and protects the open-source character of QE
- raises funds to foster the QE project and its development

Current members of the Foundation:
SISSA, EPFL, ICTP, IOM-CNR, Cineca, North Texas University, Oxford University

Users' community: factoids

- 1600+ registered users for the users' mailing list
- An average of $\sim$ 8 messages a day on the mailing list
- 6.2 version downloaded 9500 times in less than two months [*]
- 30+ Schools or tutorials since 2002, attended by $\sim$ 1200 users
- 4 developers' schools since 2013, latest in 2017
- Annual developers' meeting since 2010

[*] Number may be inflated by bots, failed or repeated downloads, etc.

Quantum ESPRESSO as a distribution

QE is not a monolithic code, it is composed of several packages:

- `PWscf`: self-consistent electronic structure, (variable-cell) structural optimization, molecular dynamics
- `CP`: Car-Parrinello molecular dynamics, also with variable cell

They share a common installation method, input format, pseudopotential 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.)
- `PWneb`: Nudged Elastic Band (NEB) for reaction pathways and barriers
- `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
- `XSpectra`: Calculation of X-ray near-edge adsorption spectra (XANES)
- `GWL`: GW band structure with ultralocalized Wannier functions
- `TD-DFPT`: Time-Dependent Density-Functional Perturbation Theory
- `EPW`: Electron-phonon coefficients and related properties

Separately distributed:

- `GIPAW`: Gauge-Independent PAW method for EPR and NMR chemical shifts
- `thermoPW`: Quasi-harmonic calculations
- `D3Q`: Anharmonic phonons

Organization

The distribution is maintained as a git public repository on `Gitlab.com`. Everybody registered on `Gitlab.com` can propose changes via the "merge request" mechanism.

- *Web site:* `www.quantum-espresso.org`
- *Developers' portal:* `gitlab.com/QEF/q-e`, mirrored at: `github.com/QEF/q-e`
- *Users' Mailing lists:* `users@lists.quantum-espresso.org`
  Only subscribed users can post. Searchable archives available at
  `https://www.mail-archive.com/users@lists.quantum-espresso.org/`
- *Developes' Mailing lists:* `developers@lists.quantum-espresso.org`
  Posts by non-subscribed users are approved if relevant

What can Quantum ESPRESSO do?

QE can be used for

- both $\Gamma-$point and **k**-point (periodic) 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 (with some limitations)
- almost all LDA and GGA functionals (PW91, PBE, B88-P86, BLYP,...), DFT+U, hybrid functionals (PBE0, B3LYP, HSE), nonlocal vdW functionals, Grimme's DFT-D, Tkatchenko-Scheffler, XDM, some meta-GGA (TPSS, SCAN)
- magnetic systems with LSDA or noncolinear magnetization, 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 (MPI) is performed on both PW's and FFT grids, using a parallel 3D FFT algorithm having good load balancing and CPU and memory scaling

- Further parallelization levels:
  – on **k**-points ("pools")
  – on NEB configurations, phonon modes ("images")
  – on bands in FFT ("task groups") and in exact exchange
  – on linear algebra: distributed parallel orthonormalization or diagonalization
  – OpenMP parallelization

Technical characteristics (coding)

- written in modern (F2003) Fortran, with various degrees of sophistication (i.e. use of advanced Fortran 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.
- OpenMP parallelization is also present

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

Data file format

New data format for easy data exchange between different codes:

- an XML file containing input data, computational details, main output data (e.g. energy, forces, structure)
- binary files, optionally in portable HDF5 format, for the charge density and Kohn-Sham orbitals (one file per **k**-point).

XML file read and written using the `FoX` library. Advantages:

- *efficient*: binary I/O for large data records
- *extensible*: based on “fields” introduced by XML syntax
  `<field> ... </field>`
- *easy* to read, write, and understand
- syntax can be *validated* via the XML “schema”

Pseudopotentials

PP's must be given in one of the following formats:

- UPF (Unified Pseudopotential Format) v.2:
  - formatted (small amount of data)
  - human-readable (may contain info needed to reproduce the PP)
  - extensible (XML syntax)
  - documented (partially)
  - converters from many other formats are available
- Deprecated but still accepted old formats:
  - Old UPF v.1
  - Old norm-conserving PP format, semilocal form, 1 projector per ℓ
  - Old format for ultrasoft and norm-conserving PP's with ≥ 1 projectors per ℓ
  - David Vanderbilt's format for ultrasoft PP's

Coming soon: XML format with schema

Table of PP available at `pseudopotentials.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
- Electronic and ionic minimization schemes: damped dynamics, conjugate gradient
- Verlet dynamics with mass preconditioning
- Variable-cell Car-Parrinello-Rahman dynamics
- Temperature control: Nosé thermostat for electrons, ions, cell; velocity rescaling
- Constrained dynamics

CP/FPMD package, advanced features

- Modified kinetic functional for constant-pressure calculations
- Metallic systems: ensemble (variable-occupancy) dynamics
- Self-Interaction Correction for systems with one unpaired electron
- Dynamics with Wannier functions under an external electric field
- Fast hybrid functionals with maximally localized Wannier functions
- Finite electric fields with Berry's phase

Not implemented: PAW, **k** points, noncollinear magnetism

PWscf package

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

- Self-consistent ground-state energy and Kohn-Sham orbitals, forces, structural optimization also with variable cell
- 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
- Hybrid functionals with fast calculation of exact exchange using localization

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)
- STM maps
- Electron Localization Function (ELF)
- Planar averages
- Density of states (DOS), projected DOS
- Interfaces with external codes

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

Pseudopotentials can be generated for all LDA/GGA Functionals that are implemented in QE (no meta-GGA, vdW-DF, hybrid functionals)

Authors

Contributors to QE, in addition to the authors of the documenting papers, are listed in the section `People` of the general user guide and of package-specific user guides. **Thanks to all of them!**