QUANTUM ESPRESSO FOUNDATION

QUANTUMESPRESSO

Efficient materials modelling on HPC
with QUANTUM ESPRESSO, Yambo and BigDFT

The QUANTUM ESPRESSO suite

Brief overview

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(SISSA)

MAX

CINECA

ENCCS
EuroCC National Competence Centre Sweden

EPFL

MARVEL
NATIONAL CENTRE OF COMPETENCE IN RESEARCH

Swiss National Science Foundation

QUANTUM ESPRESSO

- QUANTUM ESPRESSO is Quantum op**E**n-**S**ource **P**ackage for **R**esearch in **E**lectronic **S**tructure **S**imulation and **O**ptimization
- exists since 2002, resulting from the merge of pre-existing packages; some core components have been under development for ~ 30 years
  - **PWscf** and **PHonon** (Baroni, De Gironcoli, Dal Corso, Giannozzi and others …)
  - **CP/FPMD** (Pasquarello, Laasonen, Trave, Car, Marzari, Cavazzoni, Scandolo and others …)
- Main goals of QUANTUM ESPRESSO are:
  - **innovation** in theoretical methods and numerical algorithms
  - **efficiency** on modern computer architectures

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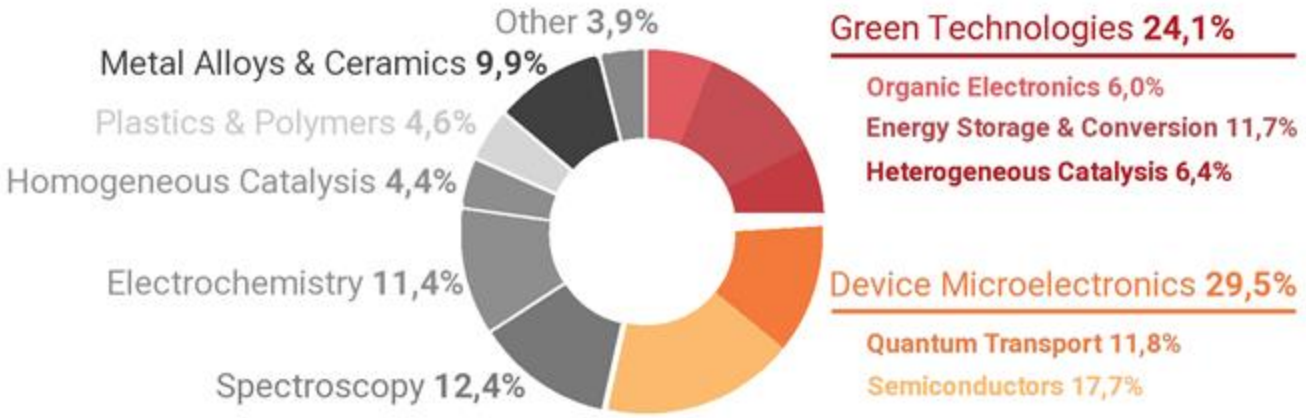
Standard open-source package for DFT calculations with plane-waves and pseudopotentials:



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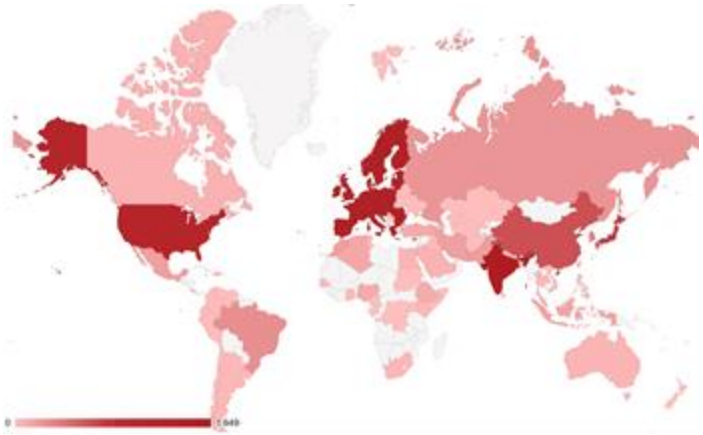
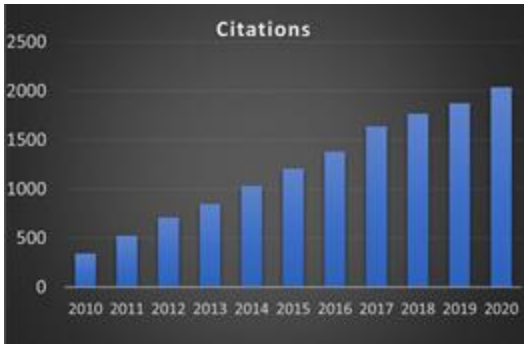
- Involves a large community of developers from different regions of the world.

- 20000 total citations

- About 30000 download in 2022





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The Suite:

Libraries:

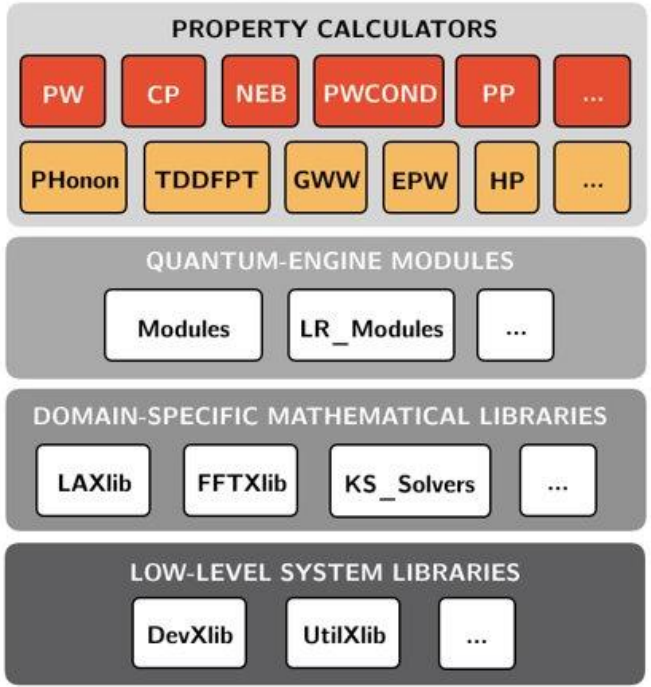
- Completely encapsulated can be easily reused in other codes.
- Are distributed by the MAX centre.

Modules:

- Encapsulated and self contained but still dependent on Q.E. datastructure
- Mostly fitted to be used for internal development in Q.E. of packages with similar data structure

Applications:

- Quantum engines
- Property calculators



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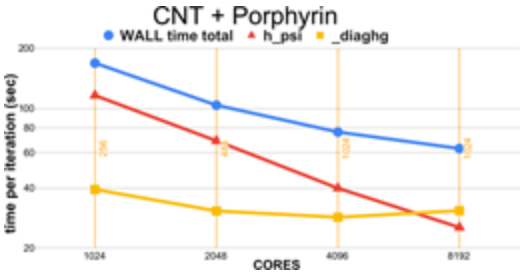
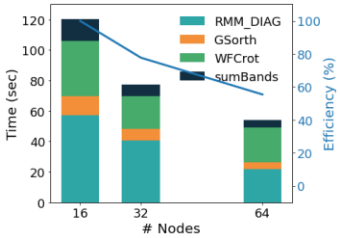
The Applications:

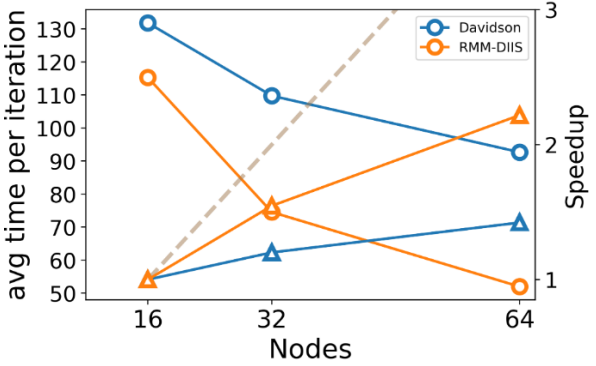
- PWscf:
  - Total energies, forces stresses using plane waves + pseudopotentials or PAW
  - L(S)DA , GGA , metaGGA and many other advanced functionals
  - collinear and noncollinear spin density
  - much more …
- CP - Car-Parrinello molecular dynamics
- NEB – Nudged elastic band
- PHonon: vibrational frequencies, dielectric response, anharmonic terms and many more with linear response
- HP - Computes Hubbard parameters with linear response
- TDDFPT: Optical spectra and collective excitations.
- QEHeat: energy flux.
- PP: post-processing utilities
- EPW: electron phonon with Wannier Function
- KCW: Koopmans-Compliant band structure calculations with Wannier Functions
- Interoperability with many other external packages …

Performance

- R&G MPI group
  - distributes 3D FFT data, scalar 1D and 2D Fourier Transforms, BLAS and loop operations on wave-function components
  - Efficient up to ~ 1/3 of FFT grid dimension
  - R&G groups can be duplicated to work distinct group of bands (task-groups)
- Parallel linear algebra
  - Dense diagonalization in the iterative space become the bottleneck for large systems.
  - KS_SOLVER provides, better scaling alternatives
- Additional parallelization levels (pools, bands)







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Performance Portability: the GPU case

- Most of the parallelization at the R&G level is distributed on within the GPU
    - Loops and BLAS call are straightforward
    - 3D FFTs are executed in batched mode, overlapping computation and communication
- The matrices in the iterative space are not distributed. All work done on one GPU
- Size of R&G groups chosen to reduce the memory per GPU.
    - Efficient parallelization only with the auxiliary levels (pools, bands)

PW:

- SCF calculations:
  - spin-degenerate, spin-polarized, noncollinear (+SOC)
  - Standard DFT functionals
  - metaGGA
  - Non-local functionals
  - Hubbard (onsite and intersiate) corrections
  - Hybrid Functionals
- Forces and Stress
  - Relaxations
  - NEB
  - Molecular dynamics
- Isolated systems
  - Clusters and Surfaces
  - Dipole corrections for 2D system
- Electric Fields
- …

The pseudopotentials:

- QE applications use pseudotentials in the UPF format.
- Possible to use Norm-Conserving and for most functionalities Ultra-Soft and PAW.
- Places where to find pseudos:
  - SSSP(https://www.materialscloud.org/discover/sssp/table/efficiency)
  - Pslibrary (https://dalcorso.github.io/pslibrary/)
  - PseudoDojo (http://www.pseudo-dojo.org/index.html)

Other links and Pslibrary tables on
http://pseudopotentials.quantum-espresso.org/

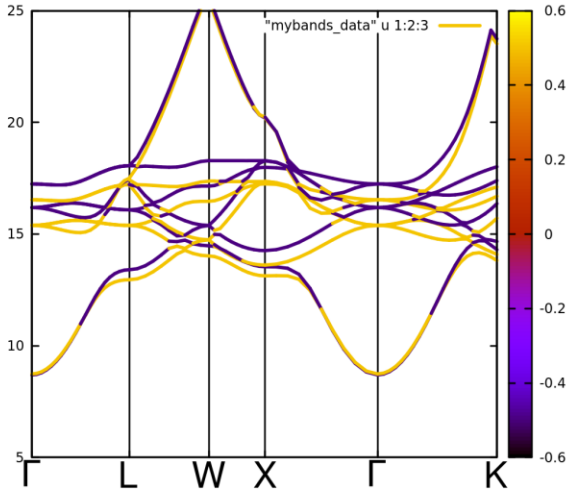
Output of PW

- Standard output: contains all results, information and warnings. No strict rule for the format.
- `prefix.save` directory contains:
  - XML data file with all results and information to reproduce/restart the run
  - charge density file (either `.dat` of `.hdf5`)
  - wave functions' files -one per k-point and spin- (either `.dat` or `.hdf5`)

Workflows for band-structure calculations

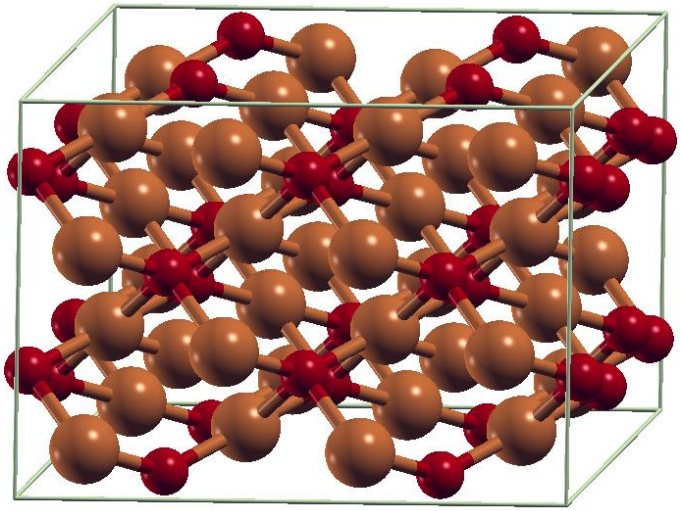
For basic band structure calculations PW functionalities are integrated with those of post-processing utilities, for example for computing Kohn-Sham bands:

1. An SCF calculations with PW:
2. A non-SCF calculation with PW
3. The post-processing utility `bands.x` performs the symmetry analysis and save the data for the plot.



Input of PW:

- The input is organized in a group of Fortran namelists + some formatted cards



```
&control
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    restart_mode = 'from_scratch'
    outdir='./out'
    pseudo-dir='pseudo'
    outdir='./'
 /
 &system
    ibrav = 0, nat=64, ntyp=2,
    ecutwfc = 35,
    ecutrho = 350,
    smearing='mp',
    occupations='smearing',
    degauss=0.01,
    nspin=2,
    starting_magnetization(1)=0.0,
    starting_magnetization(2)=0.5,
 /
 &electrons
    mixing_beta = 0.5,
    conv_thr =  1.0d-7,
    startingpot='atomic',
    startingwfc='atomic',
    electron_maxstep=4
 /

 &ions
 /

 &cell
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    press = 0
 /

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  Cu 1.0 cu_pbe_v1.2.uspp.F.UPF

CELL_PARAMETERS angstrom
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        0.0000000000         6.8406000137         0.0000000000
       -1.7280819494         0.0000000000        10.1022633844

ATOMIC_POSITIONS crystal
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   O  0.000000000         0.791500000         0.875000000
   O  0.000000000         0.791500000         0.375000000
   O  0.250000000         0.458500000         0.125000000
   O  0.250000000         0.041500000         0.875000000
```

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More info

- about QUANTUM ESPRESSO
  - Web: www.quantum-espresso.org
  - Downloads: https://www.quantum-espresso.org/download-page/
  - papers:
    - P. Giannozzi *et al.*, J.Phys.:Condens.Matter **21**, 395502 (2009) http://dx.doi.org/10.1088/0953-8984/21/39/395502
    - P. Giannozzi *et al.*, J.Phys.:Condens.Matter **29**, 465901 (2017) http://iopscience.iop.org/article/10.1088/1361-648X/aa8f79
    - P. Giannozzi et al. J. Chem. Phys. **152**, 154105 (2020); https://doi.org/10.1063/5.0005082

- about QEF foundation.quantum-espresso.org
- Development on gitlab.com/QEF/q-e

Thanks !!!

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