

# Introduction to Quantum-Espresso

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QUANTUMESPRESSO

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# Outline

- 1 Introduction
- 2 The input
  - Namelists
  - Cards
- 3 Data analysis

# Web-site introduction



Quantum ESPRESSO is an integrated suite of computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials (both norm-conserving and ultrasoft).

Source : <http://www.quantum-espresso.org/>

- **ESPRESSO** = op**E**n **S**ource **P**ackage for **R**esearch in **E**lectronic **S**tructure, **S**imulation, and **O**ptimization
- GNU General Public License

- Codes under Quantum ESPRESSO
  - PWSCF : Plane-wave self-consistent field
  - PP: Post-processing
  - CP : Car-Parrinello molecular dynamics
  - PHONON : Phonon calculations
  - FPMD : Molecular Dynamics
  - Wannier
- We'll mostly deal with PWSCF (pw.x). Other components have similar input structure.

# Capabilities

- Self-consistent, planewave, pseudopotential total energy calculation
- Large xc library : LDA, GGA, BLYP, LDA+U
- Pseudopotential-generation code and pseudopotential library
  - Norm-conserving, ultrasoft
  - Scalar relativistic, fully relativistic

]

text

- Geometric optimization also with variable cells
- Phonon calculations, (harmonic/anharmonic/e-ph)
- Inclusion of electric field, macroscopic polarizability
- Noncollinear magnetism
- Infrared and Raman cross sections
- Dielectric tensors
- Metadynamics
- Ballistic conductance
- Maximally localized Wannier functions
- Nudged Elastic Bands (NEB)



- Pros :

- Free  $\Rightarrow$  huge community
- Mature code, core is mostly well-tested
- MANY options, keywords
- Excellent mailing list, helpful developers

- Cons :

- 
- Hard to read the code
- Redundancies/obsolete keywords

# General structure

- The input file is broken down into sections

## Namelists — calculation specifications

&CONTROL: general variables controlling the run

&SYSTEM: structural information on the system under investigation

&ELECTRONS: electronic variables

&IONS (optional): ionic variables

&CELL (optional): variable-cell dynamics

&PHONON (optional): information required to produce data for phonon calculations

# General structure

## Nonoptional and optional cards

ATOMIC SPECIES

ATOMIC POSITIONS

K\_POINTS

CELL PARAMETERS(optional)

OCCUPATIONS(optional)

FIRST\_IMAGE(optional)

LAST\_IMAGE(optional)

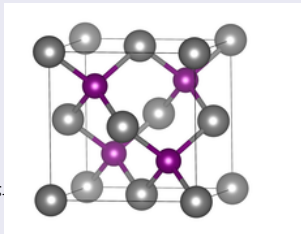
CLIMBING IMAGES(optional)

## Typical input file — diamond GaAs

```
&CONTROL
calculation = 'scf' ,
outdir = './' ,
pseudo_dir = './' ,
prefix = 'GaAs1' ,
tprnfor = .true. ,
/
&SYSTEM
ibrav = 2,
celldm(1) = 10.866264585,
nat = 2, ntyp = 2,
ecutwfc = 30 , ecutrho = 240 ,
occupations = 'smearing' ,
/
&ELECTRONS
electron_maxstep = 200,
conv_thr = 1.0D-7 ,
mixing_mode = 'plain' , mixing
mixing_ndim = 10,
diagonalization = 'david' ,
/
ATOMIC_SPECIES
Ga 69.72 ga_pbe_v1.4.uspp.F.UPF
As 74.92 as_pbe_v1.uspp.F.UPF

ATOMIC_POSITIONS crystal
Ga 0.00000 0.00000 0.00000
As 0.75000 0.75000 0.75000

K_POINTS automatics
3 3 3 0 0 0
```



# The namelist &control

## General keywords

- calculation :

scf : single point calculation without geometric optimization  
nscf : non-self-consistent calculation (needs previous  $V_{eff}(\vec{r})$ )  
relax : geometric optimization  
md : molecular dynamics  
vc-relax : geometric optimization with variable unit cell  
coordinates

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- restart\_mode :

from\_scratch : Start from an initial guess for the  $\{\psi_i(\vec{r})\}$   
restart : Start from earlier data

**Note 1** : PWSCF writes to disk  $n(\vec{r})$ ,  $V_{eff}(\vec{r})$  and  $\{\psi_i(\vec{r})\}$

**Note 2** : Must interrupt properly to resume calculation.

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- outdir : Directory where intermediates are dumped.
- pseudo\_dir : Directory where the pseudopotentials live.



# The namelist &system

## General keywords

- `nat` : number of atoms
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- `nbnd` : number of states to be calculated (unoccupied states as well)
- `ecutwfc` : kinetic energy cutoff (for planewaves)
- `ecutrho` : density cutoff (for the augmentation charge in USPP  $\approx 10 \times \text{ecutwfc}$ )

# The namelist &system

## Lattice structure

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- `ibrav` : Bravais lattice index — easy way to set up a crystal
- `celldm(1)-celldm(6)` : Various cell dimensions in B — not all six are used for most `ibrav`

0 : user-specified

1 : simple cubic

2 : face-centered cubic

3 : body-centered cubic

4 : hexagonal

⋮

Up to fourteen

`celldm(1)` = given length

`celldm(1)` =  $a$

`celldm(1)` =  $a$

`celldm(1)` =  $a$

`celldm(1)` =  $a$

`celldm(3)` =  $c/a$

⋮

Some `celldm(i)` length, some angle

# The namelist &system

## Occupations

- `occupations` : Occupation of Kohn-Sham states – important for metals
  - 'smearing' : smear occupations by a some function (below)
  - 'tetrahedra' :
  - 'fixed' : default (for insulators)
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  - 'fermi-dirac'
- degauss : Smearing width
  - Small degauss  $\Rightarrow$  better accuracy
  - Large degauss  $\Rightarrow$  smaller number of k-points



# The namelist &system

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  - 1 : non-polarized
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- `tot_magnetization` : Fix ( $n_{maj} - n_{min}$ )
- `noncolin` : (.true./false.) Turn on noncollinear magnetism

# The namelist &electrons

## Charge mixing

- `mixing_mode` : improves convergence
  - 'plain' : Broyden mixing
  - 'TF' : simple Thomas-Fermi screening (homogeneous systems)
  - 'local-TF' : local-density-dependent TF screening (surfaces etc.)
- `mixing_beta` :  $n_{i+1} = (1 - \beta)n_{i+1}^{KS} + \beta n_i$
- `mixing_nstep` : number of iterations used in mixing scheme

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## Solution of KS equations

- `diagonalization` : Minimization or iterative diagonalization
  - `david` : Davidson iterative diagonalization
  - `cg` : Minimization using the conjugate-gradients algorithm
- Various diagonalization-related keywords :
  - `diago_david_ndim`, `diago_thr_init`, `diago_cg_maxiter`

# The namelist &ions

## Ion dynamics — mostly for md

- `ion_dynamics` : Different possibilities are allowed for different calculation keywords
  - `bfgs` : for relax
  - `damp` : for relax and vc-relax
  - `verlet` : for md
- `ion_temperature` : Method of fixing the temperature during md runs
  - `'rescaling'` : rescale the velocity every given number of steps
  - `'langevin'` : use Langevin thermostat
  - `'not_controlled'` : self-evident
- NEB keywords : `opt_scheme`, `CI_scheme`, `k_min`, `k_max`

# Cards

## Related to atoms

- ATOMIC\_SPECIES

```
[ type      mass      pseudopotential ]  
  B       10.811    B.pbe-n-van.UPF  
  N       14.007    N.pbe-van_bm.UPF  
  Mn      54.938    Mn.pbe-sp-van.UPF
```

The pseudopotentials are taken from the PWSCF library or self-generated.



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```

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- ATOMIC\_POSITIONS {alat|bohr|crystal|angstrom}

```
[type      x        y        z      fix_x  fix_y  fix_z]  
  N      0.00      0.00      0.00      0       1       1  
  Mn     1.00      1.00      1.00  
  B      2.25      2.25      2.25      1       0       1
```

# Cards

## Others

- K\_POINTS { automatic }  
[ nkx    nky    nkz    shiftx   shifty   shiftz ]  
    6      6      6      0       1      0
- K\_POINTS { tpiba | crystal | gamma }  
[ k\_x       k\_y       k\_z       wk ]  
  0.25       0.25       0.25       0.333  
  0.75       0.25       0.00       0.666
- CELL\_PARAMETERS  
    a(1,1) a(2,1) a(3,1)  
    a(1,2) a(2,2) a(3,2)  
    a(1,3) a(2,3) a(3,3)  
Bohr if cellldm(1)=0, alat units otherwise

# Post-processing

- Suite of codes that take in the output  $\psi_i(\vec{r})$ ,  $V_{eff}(\vec{r})$  and  $\epsilon_i$ 's and produces various kinds of post-processed data
- Each post-processing routine has its own input.

```
&inputpp
/
&plot
    nfile = 3
    filepp(1) = "Rh100+C60.charge"
    filepp(2) = "C60.charge"
    filepp(3) = "Rh100.charge"
    weight(1) = 1.0
    weight(2) = -1.0
    weight(3) = -1.0
    iflag = 3
    output_format = 5
/
```

# What are the available post-processing routines?

- DOS, PDOS, LDOS, ILDOS
- Charge density
- STM images
- Total potential, plane-averaged potential
- Band structure
- Electron localization function
- $|\psi_i(\vec{r})|^2$