Quantum-Espresso

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Outline

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 = opEn Source Package for Research in Electronic Structure, Simulation, and Optimization
- GNU General Public License

- Codes under Quantum ESPRESSO
  - PWSCF : Plane-wave self-consisten field
  - CP : Car-Parrinello molecular dynamics
  - PHONON : Phonon calculations
  - FPMD : Molecular Dynamics
  - Wannier
- We'll mostly deal with PWSCF. Other components have similar input structure.
- Basic knowledge of atomic and solid state physics is assumed throughout the talk.

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
- 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 ⇒ huge community
  - Mature code, core is mostly well-tested
  - MANY options, keywords
  - Excellent mailing list, helpful developers
- Cons :
  - Poorly commented, user guide not great
  - 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 Si

```
 &control
    calculation = 'scf'
    restart_mode='from_scratch',
    pseudo_dir = '~/pseudo',
    outdir='tmp', /
 &system
    ibrav = 2,
    celldm(1) = 11.0,
    nat = 2,
    ntyp = 1,
    ecutwfc = 20, /
 &electrons /
ATOMIC_SPECIES
Si 1.0 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS {alat}
Si 0 0 0
Si 0.25 0.25 0.25
K_POINTS {automatic}
6 6 6 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`

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- `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 $\approx 10\times$ `ecutwfc`)

The namelist &system

Lattice structure

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Lattice structure

- `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	`celldm(1)` = given length
1 : simple cubic	`celldm(1)` = a
2 : face-centered cubic	`celldm(1)` = a
3 : body-centered cubic	`celldm(1)` = a
4 : hexagonal	`celldm(1)` = a
	`celldm(3)`=c/a
⋮	⋮
Up to fourteen	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' :
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- degauss : Smearing width

  Small degauss $\Rightarrow$ better accuracy

  Large degauss $\Rightarrow$ smaller number of k-points

The namelist &system

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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` : $n_{i+1} = (1-\beta)n^{KS}_{i+1} + \beta n_i$
- `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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- `ATOMIC_SPECIES`

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    Mn    54.938   Mn.pbe-sp-van.UPF
```

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

- `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 `celldm(1)=0`, `alat` units otherwise

Post-processing

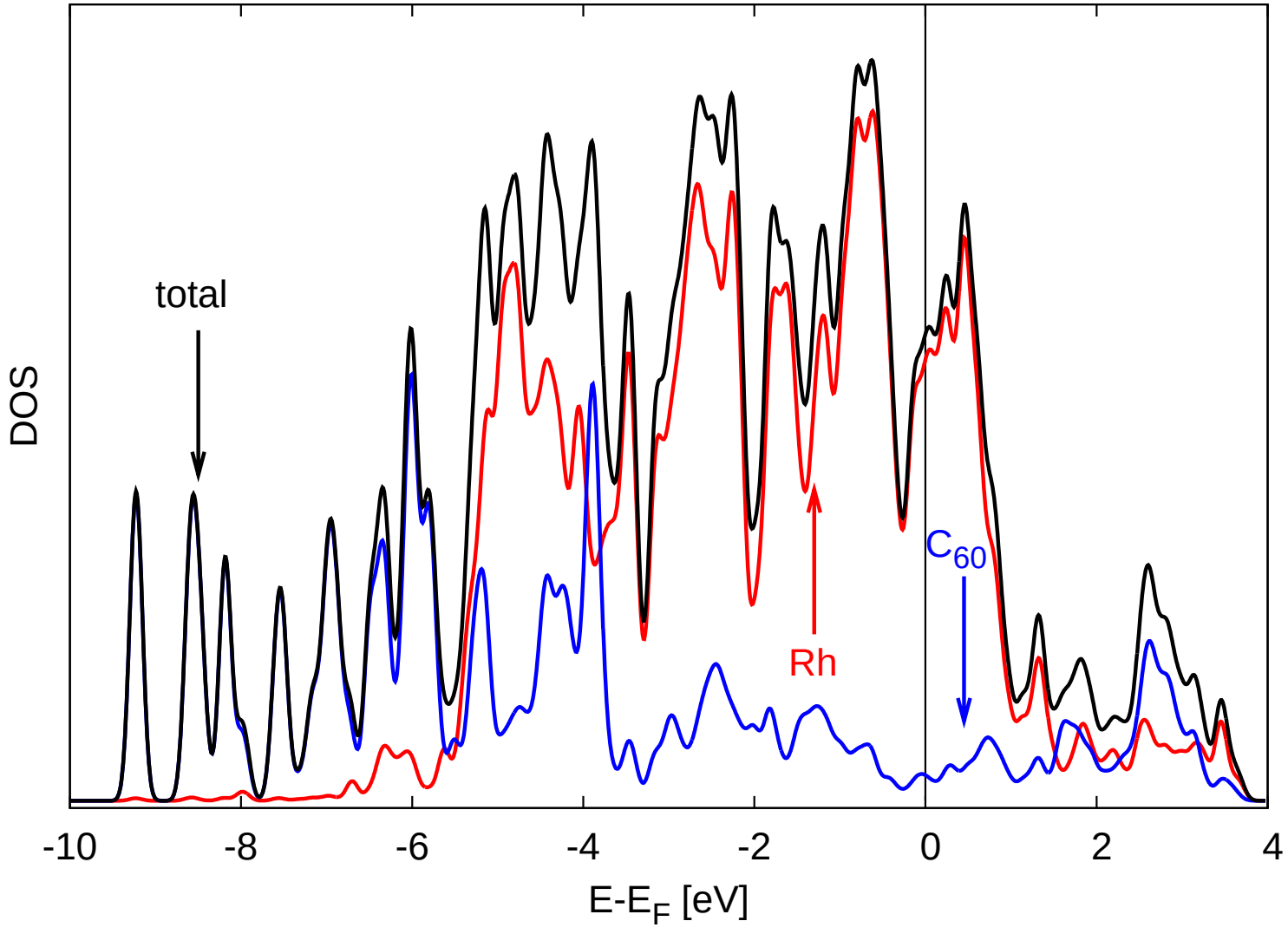
- Suite of codes that take in the output $\psi_i(\vec{r})$, $V_{eff}(\vec{r})$ and ϵ_i's and produces various kinds of post-processed data
- Each post-processing routine has its own input.

```
&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
 /
```

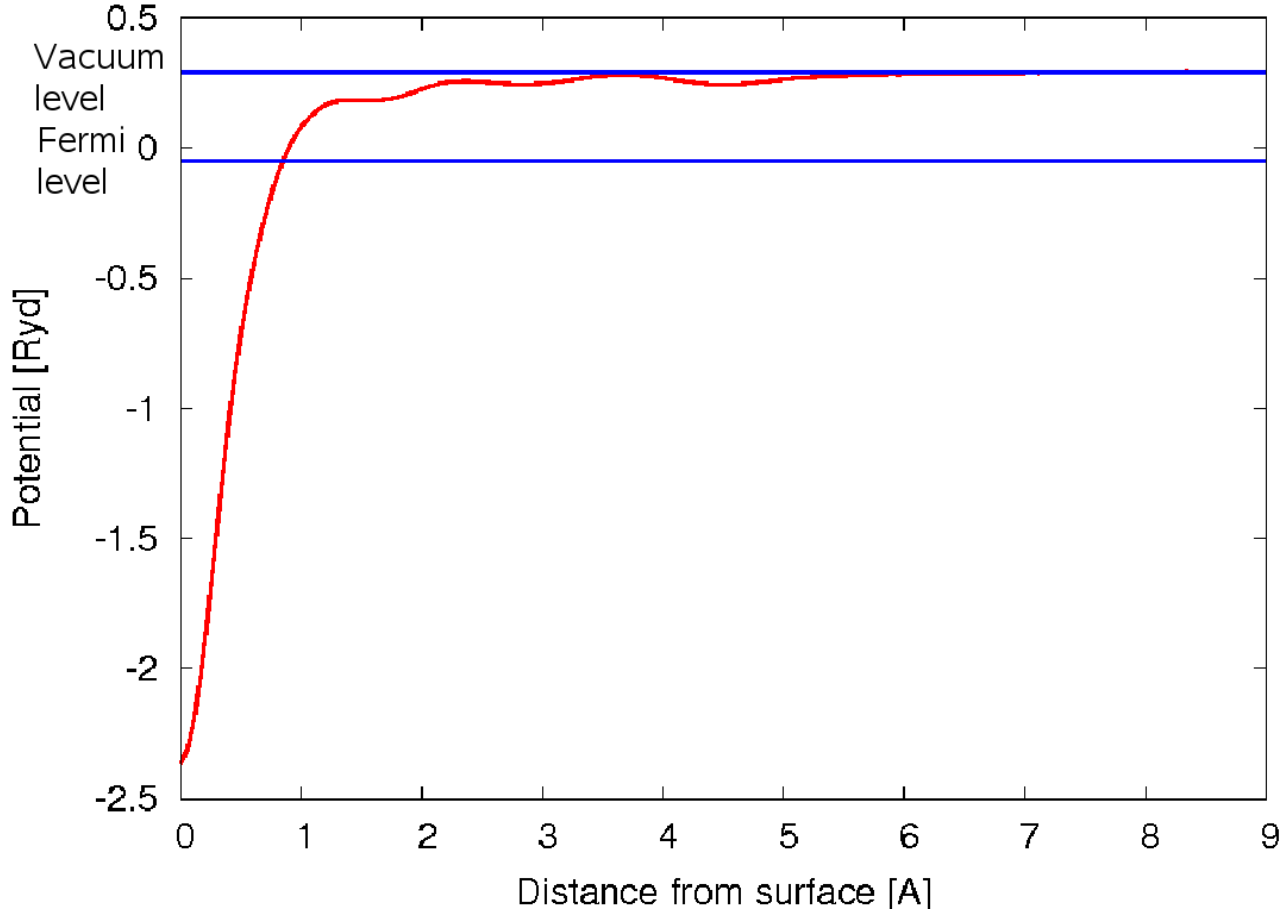
What are the available post-processing routines?

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

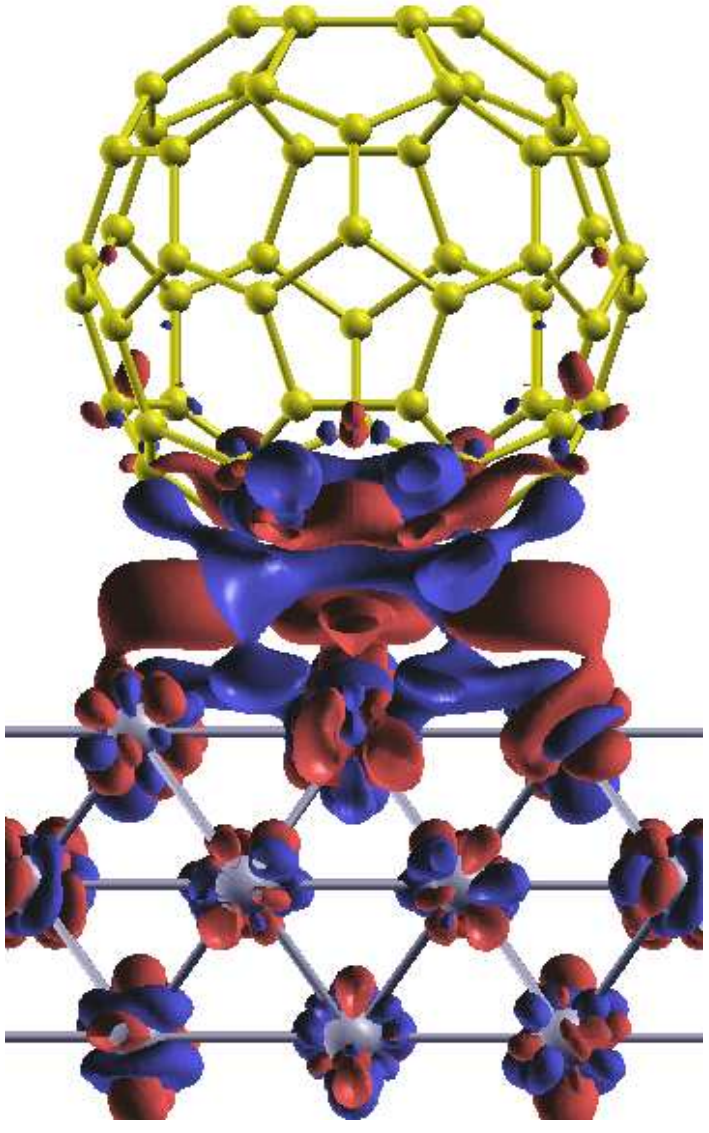
Total and partial density of states



Plane-averaged effective potential



Charge density — isosurface



Charge density — contour