# Quantum-Espresso

Hande Üstünel

25 May 2007

# 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 $\Rightarrow$ 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

# 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

- `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.

# 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
- `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.
- `outdir` : Directory where intermediates are dumped.

# 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
- `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.
- `outdir` : Directory where intermediates are dumped.
- `pseudo_dir` : Directory where the pseudopotentials live.

# The namelist `&system`

## General keywords

- `nat` : number of atoms
- `ntyp` : number of types of atoms

# The namelist &system

## General keywords

- `nat` : number of atoms
- `ntyp` : number of types of atoms
- `nbnd` : number of states to be calculated (unoccupied states as well)

# The namelist `&system`

## General keywords

- `nat` : number of atoms
- `ntyp` : number of types of atoms
- `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

- `ibrav` : Bravais lattice index — easy way to set up a crystal

# The namelist &system

## 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'` :
  - `'fixed'` : default (for insulators)
  - `'from_input'` : read occupations from a file

# 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)
  - `'from_input'` : read occupations from a file
- `smearing` : types of smearing
  - `'gaussian'`
  - `'methfessel-paxton'`
  - `'marzari-vanderbilt'`
  - `'fermi-dirac'`

# 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)
  - 'from_input' : read occupations from a file
- smearing : types of smearing
  - 'gaussian'
  - 'methfessel-paxton'
  - 'marzari-vanderbilt'
  - 'fermi-dirac'
- degauss : Smearing width
  - Small degauss ⇒ better accuracy
  - Large degauss ⇒ smaller number of k-points

# The namelist &system

## Magnetism

- `nspin` : spin type

    1 : non-polarized
    2 : spin-polarized (single-axis magnetization)

# The namelist &system

## Magnetism

- `nspin` : spin type

  1 : non-polarized

  2 : spin-polarized (single-axis magnetization)

- `starting_magnetization (i)` : between -1 and 1. To break symmetry for the initial configuration. The index `i` runs over atom types.

# The namelist &system

## Magnetism

- `nspin` : spin type

  1 : non-polarized

  2 : spin-polarized (single-axis magnetization)

- `starting_magnetization (i)` : between -1 and 1. To break symmetry for the initial configuration. The index `i` runs over atom types.

- `tot_magnetization` : Fix ($n_{maj}$ - $n_{min}$)

# The namelist &system

## Magnetism

- nspin : spin type

  1 : non-polarized
  2 : spin-polarized (single-axis magnetization)

- starting_magnetization (i) : between -1 and 1. To break symmetry for the initial configuration. The index i runs over atom types.
- 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

# 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

## 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.

# 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.

- 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

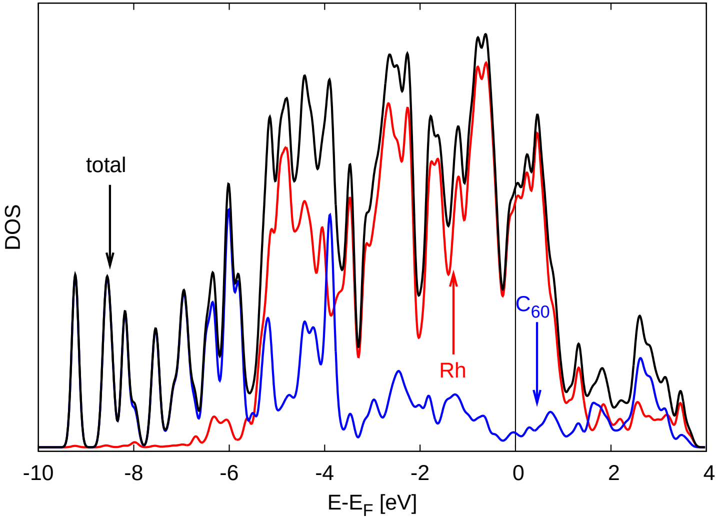
- Suite of codes that take in the output $\psi_i(\vec{r})$, $V_{eff}(\vec{r})$ and $\epsilon_i$'s and produces various kinds of post-processed data
- Each post-processing routine has its own input.

```
&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
 /
```

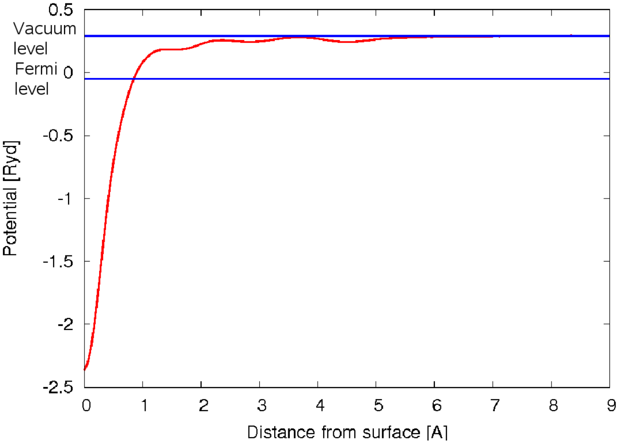
# What are the available post-processing routines?

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

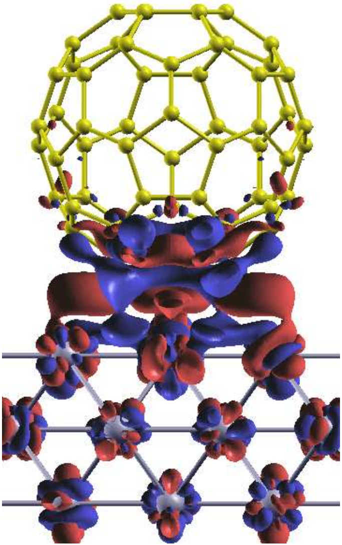
# Total and partial density of states



# Plane-averaged effective potential



# Charge density — isosurface



# Charge density — contour