Quantum Espresso Tutorial

Hands-on Session #1

First steps with QE: total energy and relaxations

Simone Piccinin
CNR – Institute of Materials (IOM), Trieste (Italy)
piccinin@iom.cnr.it
http://www.quantum-espresso.org/


QUANTUM ESPRESSO

is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modelling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.
Structure of QE input file

```plaintext
&control
  calculation = 'scf',
  prefix = 'Si_exc1',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
  Si 28.086  Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1
```
Structure of QE input file

&control
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  prefix = 'Si_exc1',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
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  ecutwfc = 20
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  mixing_beta = 0.7
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  Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1
The Kohn-Sham problem

KS eqns: \[
\left[ -\frac{1}{2} \nabla^2 + V_{\text{nucl}}(r) + V_H[n] + V_{xc}[n] \right] \Psi_i(r) = \epsilon_i \Psi_i(r)
\]

SCF: $\Psi_i(r) \rightarrow n(r) \rightarrow H[n]$
Iterative solution of KS equations

1. Construct $V_{\text{nucl}}(r)$
2. Initial guess $n(r)$
3. Compute $V_H[n] + V_{xc}[n]$
4. $V_{\text{eff}} = V_{\text{nucl}} + V_H[n] + V_{xc}[n]$
5. Solve $\left[ -\frac{1}{2} \nabla^2 + V_{\text{eff}}(r) \right] \Psi_i(r) = \epsilon_i \Psi_i(r)$
6. Compute $n(r) = \sum |\Psi_i(r)|^2$
7. Self-consistent?
   - No
   - Yes: Energy/Forces
&control
    calculation = 'scf',
    prefix = 'Si_exc1',
/
&system
    ibrav = 2,
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    nat = 2,
    ntyp = 1,
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    mixing_beta = 0.7
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    6 6 6 1 1 1
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ATOMIC_POSITIONS (alat)
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1

= 'scf', 'nscf', 'relax', 'md', ...

\&control
  calculation = 'scf',
  prefix = 'Si_exc1',
/
\&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
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  mixing_beta = 0.7
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K_POINTS (automatic)
  6 6 6 1 1 1
Iterative solution of KS equations

1. Construct $V_{nucl}(r)$
2. Initial guess $n(r)$
3. Compute $V_H[n] + V_{xc}[n]$
4. $V_{eff} = V_{nucl} + V_H[n] + V_{xc}[n]$
5. Solve $\left[ -\frac{1}{2} \nabla^2 + V_{eff}(r) \right] \Psi_i(r) = \varepsilon_i \Psi_i(r)$
6. Compute $n(r) = \sum |\Psi_i(r)|^2$
7. Self-consistent? (No/Yes)
8. Yes: Energy/Forces

Diagram:
- Start with $V_{nucl}(r)$
- Compute $V_H[n] + V_{xc}[n]$
- Use $V_{eff} = V_{nucl} + V_H[n] + V_{xc}[n]$
- Solve the Schrödinger equation
- Compute $n(r) = \sum |\Psi_i(r)|^2$
- Check self-consistency (No/Yes)
- If Yes, report Energy/Forces
Periodic Boundary Conditions

Periodic system: \textit{lattice} + \textit{basis}
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  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1

ibrav = 1: simple cubic
ibrav = 2: fcc
ibrav = 4: hexagonal
...

simple cubic:
  v1 = a(1,0,0), v2 = a(0,1,0), v3 = a(0,0,1)

fcc:
  v1 = (a/2)(-1,0,1), v2 = (a/2)(0,1,1), v3 = (a/2)(-1,1,0)

hexagonal:
  v1 = a(1,0,0), v2 = a(-1/2,\sqrt{3}/2,0), v3 = a(0,0,c/a)
Structure of QE input file

```
&control
  calculation = 'scf',
  prefix = 'Si_exc1',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
  Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1
```

fcc:

\[ v1 = \left(\frac{a}{2}\right)(-1,0,1), \quad v2 = \left(\frac{a}{2}\right)(0,1,1), \quad v3 = \left(\frac{a}{2}\right)(-1,1,0) \]
Structure of QE input file

&control
  calculation = 'scf',
  prefix = 'Si_exc1',
/
&system
  ibrav = 2,
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ATOMIC_POSITIONS (alat)
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1

Units: bohr (1 bohr = 0.529177 Å)
Structure of QE input file

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/
&system
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  ntyp = 1,
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&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 6 1 1 1

fcc:
  v1 = (a/2)(-1,0,1),  v2 = (a/2)(0,1,1),  v3 = (a/2)(-1,1,0)
```
Structure of QE input file

&control
  calculation = 'scf',
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/
&system
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  celldm(1) = 10.26,
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  mixing_beta = 0.7
/
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Si 28.086  Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
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ATOMIC_POSITIONS (alat)
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/
ATOMIC_SPECIES
  Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1
```

Name of the PP file

**NB:** If PP files are in a separate directory then specify:

```plaintext
&control
  pseudo_dir='/where/my/pseudos/are'
/
```
Structure of QE input file

```
&control
  calculation = 'scf',
  prefix = 'Si_exc1',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
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&electrons
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/
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ATOMIC_POSITIONS (alat)
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1
```

(alat, bohr, angstrom, crystal)
Iterative solution of KS equations

1. Construct $V_{nuc}(r)$
2. Initial guess $n(r)$
3. Compute $V_H[n] + V_{xc}[n]$
4. $V_{eff} = V_{nuc} + V_H[n] + V_{xc}[n]$
5. Solve $\left[-\frac{1}{2}\nabla^2 + V_{eff}(r)\right] \Psi_i(r) = \epsilon_i \Psi_i(r)$
6. Compute $n(r) = \sum |\Psi_i(r)|^2$
7. Self-consistent?
   - Yes: Energy/Forces
   - No: Repeat steps 1-6
Structure of QE input file

```plaintext
&control
  calculation = 'scf',
  prefix = 'Si_exc1',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
  Si 28.086  Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1
```

startingwfc = 'atomic' (DEFAULT)
= 'random'
= 'file'
Plane wave expansion

In a periodic system we can write the KS states as a superposition of plane waves:

$$\Psi_{k,n}(r) = \frac{1}{\Omega} \sum_{G} c_{k,n}^{G} e^{i(k+G) \cdot r}$$

G’s are vectors in reciprocal space.
The sum, in principle infinite, can be truncated:

$$\frac{\hbar^2}{2m} |k + G|^2 \leq E_{cut}$$
Plane wave expansion

In a periodic system we can write the KS states as a superposition of plane waves:

$$\Psi_{k,n}(r) = \frac{1}{\Omega} \sum_G c_{k,n}^G e^{i(k+G) \cdot r}$$

$G$'s are vectors in reciprocal space. The sum, in principle infinite, can be truncated:

$$\frac{\hbar^2}{2m} |k + G|^2 \leq E_{cut}$$

**Problems:**
1) Core electrons are localized
2) Valence electrons have nodes close to the nucleus

An all-electron calculation would require high $E_{cut}$

**Pseudopotentials:** The choice of $E_{cut}$ depends on the PP
Structure of QE input file

```plaintext
&control
  calculation = 'scf',
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/
&system
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  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
  Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1
```

\[
\frac{\hbar^2}{2m} \left| \mathbf{k} + \mathbf{G} \right|^2 \leq E_{cut}
\]

Units: Ry (1 Ry = 0.5 Ha = 13.6057 eV)

For ultrasoft pseudopotentials we have also:

ecutrho = usually 8-12 * ecutwfc
Structure of QE input file

&control
  calculation = 'scf',
  prefix = 'Si_exc1',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
  Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1

Name of the PP file: **Si.pbe-rrkj.UPF**
Pseudopotentials

<PP_INFO>
Generated using Andrea Dal Corso code (rrkj3)
Author: Andrea Dal Corso  Generation date: unknown
Info: Si PBE 3s2 3p2 RKKJ3
   0  The Pseudo was generated with a Non-Relativistic Calculation
2.5000000000E+00  Local Potential cutoff radius
nl pn l occ  Rcut  Rcut US  E_pseu
3S  1  0  2.00  2.500000000000  2.600000000000  0.000000000000
3S  1  0  0.00  2.500000000000  2.600000000000  0.000000000000
3P  2  1  2.00  2.500000000000  2.700000000000  0.000000000000
3D  3  2  0.00  2.500000000000  2.500000000000  0.000000000000
</PP_INFO>

<PP_HEADER>
  0  Version Number
  Si  Element
  NC  Norm - Conserving pseudopotential
  F  Nonlinear Core Correction
  SLA PW PBE PBE  PBE Exchange-Correlation functional
  4.00000000000  Zvalence
  -7.47480832270  Total energy
  0.000000  0.000000  Suggested cutoff for wfc and rho
  2  Max angular momentum component
  883  Number of points in mesh
  2  3  Number of Wavefunctions, Number of Projectors
Wavefunctions   nl l occ
   3S  0  2.00
   3P  1  2.00
</PP_HEADER>

<PP_MESH>
<PP_R>
1.77053726905E-04  1.79729551320E-04  1.82445815642E-04  1.85203131043E-04
1.88002117930E-04  1.90843406086E-04  1.93727634813E-04  1.96655453076E-04
1.99627519645E-04  2.02644503249E-04  2.057082721E-04  2.08815947154E-04
2.1197176056E-04  2.15175339506E-04  2.18427298316E-04  2.21728404189E-04
2.25079399889E-04  2.28481039403E-04  2.31934088115E-04  2.35439322975E-04
2.38997532677E-04  2.42609517831E-04  2.46276091150E-04  2.49998077629E-04
...
PSEUDOPOTENTIALS

Ready-to-use pseudopotentials are available from the periodic table below. Choose the options you desire from the menus (pseudopotentials from PSLibrary are recommended), then press "Filter". Elements for which at least a pseudopotential is available will appear in red. Click on the element entry and follow the link to access the pseudopotentials and a minimal description of their characteristics.

More information about pseudopotentials in general, the naming convention adopted for pseudopotential files, the Unified Pseudopotential Format, and on other pseudopotential databases, can be found via the links of the menu at the left.

Important Note: although most of these pseudopotentials were published or used with satisfactory results in published work, we cannot give any warranty whatsoever that they fit your actual needs.
PSLibrary is a library of inputs for the LDL.x atomic code. It allows the generation of PWm data sets, ultrasoft, and norm conserving pseudopotentials for many elements.

Recent News

**PSLibrary 0.3.0 released**

Andrea Dal Corso
2012-10-31

PSLibrary 0.3.0 has been released.

<table>
<thead>
<tr>
<th>Time</th>
<th>Activity Type</th>
<th>By</th>
</tr>
</thead>
<tbody>
<tr>
<td>2013-Apr-05</td>
<td>18:30:24 Commits: Added an fire with the old FPs, removed from the main scripts. Added the License file.</td>
<td>Andrea Dal Corso</td>
</tr>
<tr>
<td>2013-Apr-03</td>
<td>18:25:34 Commits: The PPs of Nb, Sc, Sr, Zr, Ti seems to work. Moved from the _tot script to the main distribution. Several other minor modifications.</td>
<td>Andrea Dal Corso</td>
</tr>
<tr>
<td>2013-Apr-03</td>
<td>16:49:00 Commits: Further cleanup of the best scripts.</td>
<td>Andrea Dal Corso</td>
</tr>
<tr>
<td>2013-Apr-02</td>
<td>16:15:52 Commits: Cleanup of tests.</td>
<td>Andrea Dal Corso</td>
</tr>
</tbody>
</table>

Description

The purpose of the project is to provide a library of inputs of the LDL.x code for the generation of a standard set of norm conserving, ultrasoft and PWm pseudopotentials.

Technical Info

- Author: Andrea Dal Corso

Trove Categorization

- Development Status: Alpha
- Intended Audience: End Users/Desktop
- License: GNU General Public License (GPL)
- Topic: Density-Functional Theory calculations, Quantum ESPRESSO related
Structure of QE input file

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&system
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  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
  Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1
Sampling of the Brillouin zone

Many quantities we need to compute involve an integral over the BZ:

$$\bar{A} = \frac{1}{\Omega_{BZ}} \int_{BZ} A(k) dk$$

An example is the electronic density \(n(r)\):

$$n(r) = \frac{1}{\Omega_{BZ}} \sum_i \int_{BZ} |\Psi_{i,k}(r)|^2 f(\epsilon_{i,k} - \epsilon_F) dk$$

In practice the integral is discretized:

$$\frac{1}{\Omega_{BZ}} \int_{BZ} dk \to \sum_k \omega_k$$

How do we choose the \(k\) points to include in the sum?
Sampling of the Brillouin zone

- Example: square 2D lattice
- 4x4 k-points grid (16 points)
- 3 inequivalent points (IBZ)
  - $4 \times k_1 \rightarrow \omega_1 = \frac{1}{4}$
  - $4 \times k_2 \rightarrow \omega_2 = \frac{1}{4}$
  - $8 \times k_3 \rightarrow \omega_3 = \frac{1}{2}$

$$\frac{1}{\Omega_{BZ}} \int_{BZ} A(k) \, dk \approx \frac{1}{4} A(k_1) + \frac{1}{4} A(k_2) + \frac{1}{2} A(k_3)$$
Structure of QE input file

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  calculation = 'scf',
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&system
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  nat = 2,
  ntyp = 1,
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/
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  mixing_beta = 0.7
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  Si 28.086  Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1
```

(automatic, tpiba, crystal, gamma)
Structure of QE input file

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  Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1

Nk1, NK2, NK3, shift1, shift2, shift3
shift: 0 or 1
Sampling of the Brillouin zone

Discontinuity of occupations

\[
n(r) = \frac{1}{\Omega_{BZ}} \sum_i \int_{BZ} |\Psi_{i,k}(r)|^2 f(\epsilon_{i,k} - \epsilon_F) dk
\]

a) \( f(x) = \Theta(x) = \begin{cases} 
1 & \text{for } x \leq 0 \\
0 & \text{for } x > 0 
\end{cases} \)

b) \( f(x) = \) smooth function of \( x/\sigma \)
   (i.e. partial occupations)

\( \sigma \): dimensions of energy,
controls the broadening of the Fermi surface
“smearing” of the Fermi surface
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    Si 0.25 0.25 0.25
K_POINTS (automatic)
    6 6 6 1 1 1

occupations = ‘smearing’
smearing = ‘gaussian’
(degauss = 0.01)
(or mp, mv, fd)
(units: Ry)
Iterative solution of KS equations

1. Construct $V_{nucl}(r)$
2. Initial guess $n(r)$
3. Compute $V_H[n] + V_{xc}[n]$
4. $V_{eff} = V_{nucl} + V_H[n] + V_{xc}[n]$
5. Solve $\left[ -\frac{1}{2} \nabla^2 + V_{eff}(r) \right] \Psi_i(r) = \epsilon_i \Psi_i(r)$
6. Compute $n(r) = \sum |\Psi_i(r)|^2$
7. Self-consistent? (Yes/No)
8. Energy/Forces
Structure of QE input file

```fortran
&control
calculation = 'scf',
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/
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ATOMIC_SPECIES
Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 6 1 1 1
```

Name of the PP file: **Si.pbe-rrkj.UPF**

By default the XC functional is chosen based on the information contained in the PP file.

ntyp > 1 --> XC must be consistent (or overwritten)
Structure of QE input file

```plaintext
&control
  calculation = 'scf',
  prefix = 'Si_exc1',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
  Si 28.086  Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1
```

input_dft = 'rpbe'
  = 'pz'
  = 'b3lyp'
  = ... (see espresso-5.0.2/Modules/funct.f90)

Name of the PP file: **Si.pbe-rrkj.UPF**

By default the XC functional is chosen based on the information contained in the PP file.

ntyp > 1 --> XC must be consistent (or overwritten)
Iterative solution of KS equations

1. Construct $V_{nucl}(r)$
2. Initial guess $n(r)$
3. Compute $V_H[n] + V_{xc}[n]$
4. Solve $\left[-\frac{1}{2} \nabla^2 + V_{eff}(r)\right] \Psi_i(r) = \epsilon_i \Psi_i(r)$
5. Compute $n(r) = \sum |\Psi_i(r)|^2$
6. Check self-consistency
   - No
   - Yes: Energy/Forces
Structure of QE input file

&control
  calculation = 'scf',
  prefix = 'Si_exc1',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
  Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1

diagonalization = 'david' (DEFAULT)
  = 'cg'
Iterative solution of KS equations

1. **Construct** $V_{nucl}(r)$
2. **Initial guess** $n(r)$
3. **Compute** $V_H[n] + V_{xc}[n]$
4. **Solve** $\left[-\frac{1}{2}\nabla^2 + V_{eff}(r)\right] \Psi_i(r) = \epsilon_i \Psi_i(r)$
5. **Compute** $n(r) = \sum |\Psi_i(r)|^2$

**Self-consistent?**

- **No**
- **Yes** **Energy/Forces**
Structure of QE input file

&control
  calculation = 'scf',
  prefix = 'Si_exc1',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
  Si 28.086  Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS (automatic)
  6 6 6 1 1 1

conv_thr = 1.d-6 (DEFAULT)
= 1.d-8
Iterative solution of KS equations

Construct $V_{nucl}(r)$

Initial guess $n(r)$

Compute $V_H[n] + V_{xc}[n]$ 

$V_{eff} = V_{nucl} + V_H[n] + V_{xc}[n]$ 

Solve $\left[-\frac{1}{2} \nabla^2 + V_{eff}(r)\right] \Psi_i(r) = \epsilon_i \Psi_i(r)$

Compute $n(r) = \sum |\Psi_i(r)|^2$

Self-consistent? 

No 

Energy/Forces 

Yes

Mixing

- Mix new and old density
- 0.7 = 70% of the new density and 30% of old at first step, then use Broyden scheme

```
&control
  calculation = 'scf',
  prefix = 'Si_exc1',
/
&system
  ibrav = 2,
  celldm(1) = 10.26,
  nat = 2,
  ntyp = 1,
  ecutwfc = 20
/
&electrons
  mixing_beta = 0.7
/
ATOMIC_SPECIES
  Si 28.086 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
KPOINTS (automatic)
  6 6 6 1 1 1
```
Iterative solution of KS equations

Construct $V_{nucl}(r)$

Initial guess $n(r)$

Compute $V_H[n] + V_{xc}[n]$

$V_{eff} = V_{nucl} + V_H[n] + V_{xc}[n]$  

Solve $\left[-\frac{1}{2}\nabla^2 + V_{eff}(r)\right] \Psi_i(r) = \epsilon_i \Psi_i(r)$

Compute $n(r) = \sum |\Psi_i(r)|^2$

Self-consistent?  

Yes  

Energy/Forces

No
Iterative solution of KS equations

1. Construct $V_{nucl}(r)$
2. Initial guess $n(r)$
3. Compute $V_H[n] + V_{xc}[n]$
4. Solve
   $$\left[-\frac{1}{2} \nabla^2 + V_{eff}(r)\right] \Psi_i(r) = \epsilon_i \Psi_i(r)$$
5. Compute $n(r) = \sum |\Psi_i(r)|^2$
6. Move ions
7. Self-consistent?
   - No
   - Yes: Energy/Forces
Structure of QE input file

&control
  calculation = 'relax',
  nstep=50,
  etot_conv_thr = 1.d-4
  forc_conv_thr = 1.d-3
...
/
...
&electrons
  conv_thr = 1.d-7
...
/
&ions
  ion_dynamics = "bfgs",
  pot_extrapolation = "second_order",
  wfc_extrapolation = "second_order",
  upscale = 100,
/
...

(DEFALT: 'none')
(DEFALT: 10)
Exercises

Read the instructions !!!

Exercise 1: bulk Si
• convergence of $E_{tot}$ w.r.t. plane waves cutoff ($ecutwfc$)
• convergence of $E_{tot}$ w.r.t. BZ sampling ($K$ _POINTS)
• lattice constant

Exercise 2: bulk Al (metal!)
• convergence of $E_{tot}$ w.r.t. plane waves cutoff ($ecutwfc$)
• convergence of $E_{tot}$ w.r.t. BZ sampling ($K$ _POINTS)
• lattice constant