

# Quantum Espresso Tutorial

---

# Goal?

---

- Know what you want from the code. It is not about defining atoms and changing parameters
- Strength of DFT:
  - Energetics:** point defects formation energies, migration energies,...
  - Electronic structure:** charge localization, magnetic properties,....
- **How is it done?** Kohn- Sham equation is solved using pw.x code in QE package.

# Codes in QE package

---

PW.X

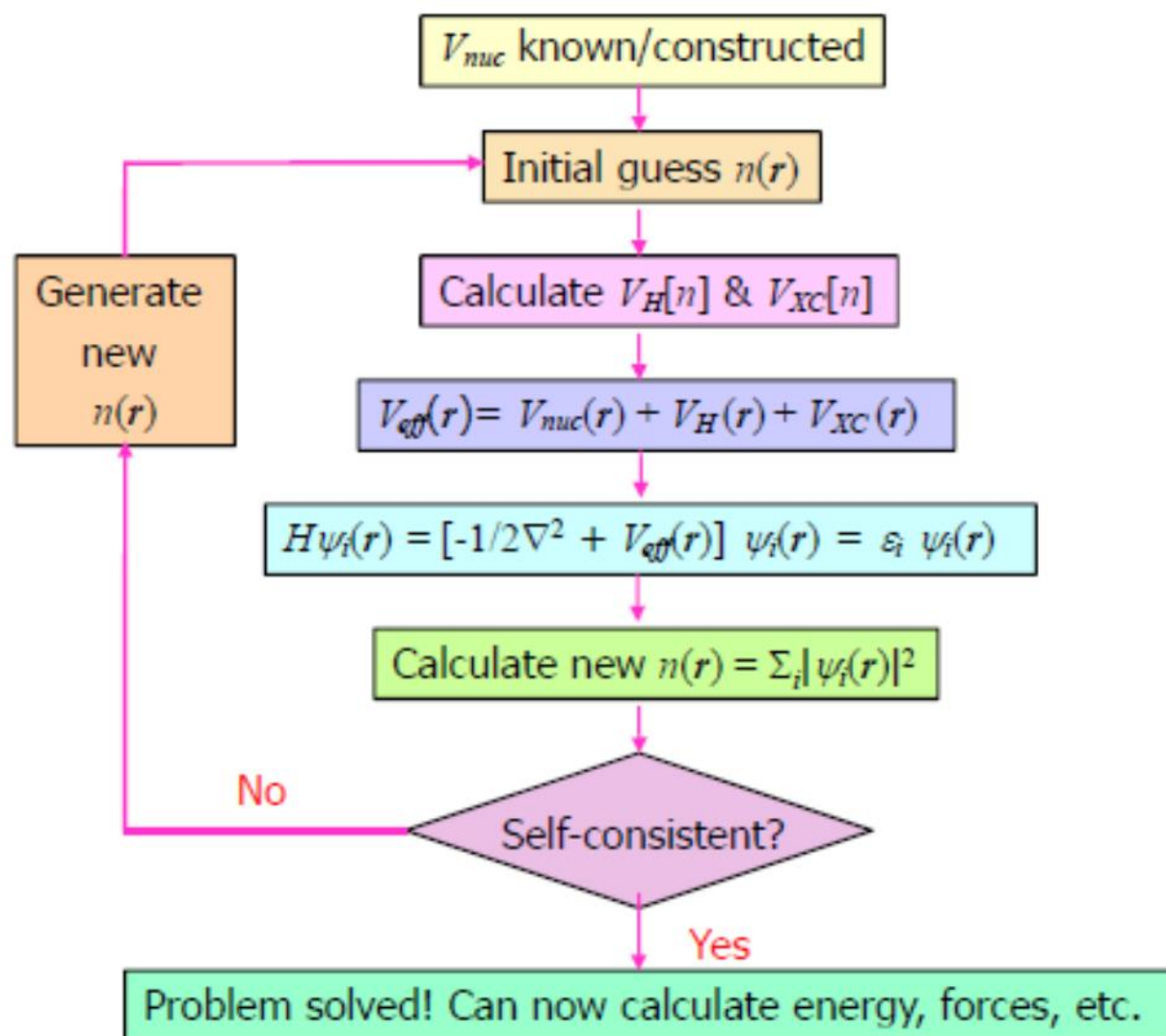
NEB.X

DOS.X

PP.X

..,etc.

# Self-consistent Iterative Solution



# Sample Input Files

---

&CONTROL

```
calculation = 'scf' ,  
prefix='Silicon' ,  
outdir='E:\Graduate\QE_tutorial\perfect\outdir' ,  
pseudo_dir = 'E:\Graduate\QE_tutorial\' ,  
/  
&SYSTEM
```

```
ibrav = 0 ,  
nat = 8 ,  
ntyp = 1 ,  
ecutwfc = 30 ,  
ecutrho = 240 ,  
/  
&ELECTRONS
```

```
/  
&IONS
```

```
/  
&CELL
```

```
/  

```

ATOMIC\_SPECIES

Si 28.086 Si.pbe-n-rrkjus\_psl.UPF

ATOMIC\_POSITIONS crystal

Si	0.000000000	0.000000000	0.000000000
Si	0.000000000	0.500000000	0.500000000
Si	0.500000000	0.500000000	0.000000000
Si	0.500000000	0.000000000	0.500000000
Si	0.750000000	0.250000000	0.750000000
Si	0.250000000	0.250000000	0.250000000
Si	0.250000000	0.750000000	0.750000000
Si	0.750000000	0.750000000	0.250000000

CELL\_PARAMETERS angstrom

5.4700000000	0.0000000000	0.0000000000
0.0000000000	5.4700000000	0.0000000000
0.0000000000	0.0000000000	5.4700000000

K\_POINTS automatic

4 4 4 1 1 1

&CONTROL	&ELECTRONS	CELL_PARAMETERS angstrom
		5.439039 0.000000 0.000000
calculation = 'relax' ,	diagonalization='david',	3.097504 4.470863 0.000000
prefix='fe2o3' ,	mixing_mode = 'plain' ,	3.097504 1.622263 4.166159
outdir='/home/data/prim_fe2o3_dft+u/scratch' ,	mixing_beta = 0.7,	
pseudo_dir = '/home/alex021u1/data' ,	startingwfc = 'random',	ATOMIC_SPECIES
etot_conv_thr = 7.7D-6 ,	conv_thr = 1.0d-9 ,	Fe1 55.845 Fe.pbe-spn-rrkjus_psl.0.2.1.UPF
forc_conv_thr = 4.0D-5 ,		
/	/	Fe2 55.845 Fe.pbe-spn-rrkjus_psl.0.2.1.UPF
&SYSTEM		
ibrav = 0 ,	&ions	O 15.999 O.pbe-n-rrkjus_psl.0.1.UPF
nat = 10,		
ntyp = 3 ,	ion_dynamics='bfgs'	ATOMIC_POSITIONS crystal
nbnd = 60 ,		Fe1 0.144983 0.144983 0.144984
ecutwfc = 90 ,	/	Fe1 0.855016 0.855016 0.855016
ecutrho = 1080 ,		Fe2 0.355016 0.355016 0.355016
occupations = 'fixed',	&CELL	Fe2 0.644983 0.644983 0.644982
nspin = 2 ,		O 0.749999 0.444610 0.055389
starting_magnetization(1)=1.0,	cell_dynamics = 'bfgs' ,	O 0.944610 0.249999 0.555389
starting_magnetization(2)=-1.0,	cell_dofree = 'all',	O 0.444610 0.055389 0.750000
tot_magnetization = 0,	press_conv_thr = 0.5 ,	O 0.249999 0.555389 0.944610
lda_plus_u = .TRUE. ,		O 0.055389 0.749999 0.444610
Hubbard_U(1) = 3.0 ,	/	O 0.555389 0.944610 0.249999
Hubbard_U(2) = 3.0 ,		
Hubbard_U(3) = 7.0 ,		K_POINTS automatic
/		8 8 8 0 0 0

# Understanding Input Parameters

---



# Namelists

---

- Must be in the following order ➔
- Start with “&” and end with “/”

```
&CONTROL  
...  
/  
&SYSTEM  
...  
/  
&ELECTRONS  
...  
/  
&IONS  
..  
/  
&CELL  
..  
/
```

# Input Parameters in “&Control”

---

- Calculation = ‘scf’, ‘relax’, ‘vc-relax’, ‘md’,..
- scf: self-consistent field (simply, calculate ground state energy and charge density)
- relax: calculate forces after each scf cycle and change ionic positions to minimize forces (but cell size is fixed)
- vc-relax: variable cell relax

# Input Parameters in “&Control”

---

- Outdir = '\$path\_to\_folder\_to\_create\_output\_files'
- pseudo\_dir= '\$path\_to\_folder\_of\_pseudopotential\_files'
- etot\_conv\_thr = convergence threshold for total energy in ionic relaxation (in Rydberg)
- forc\_conv\_thr = convergence threshold for forces in ionic relaxation (in Ry/bohr)

1 Ry = 13.6 eV

1 bohr = 0.529 Angstrom

# Input Parameters in “&System”

---

- **ibrav** = Bravais lattice index  
1: simple cubic, 2: FCC, 3: BCC, see manual for more structures

Recommended: use (**ibrav=0**) and specify lattice vectors in (CELL\_PARAMETERS) card

- **nat**: number of atoms in simulation cell
- **ntyp**: number of atomic species
- **nbnd**: number of electronic states to calculate ( $n/2$  + extra states in conduction band (20% more))

# Input Parameters in “&System”

---

- tot\_charge : (if not assigned, default = 0), used in modeling charged defects
- nspin= 1 for non-polarized calc. , 2 for spin-polarized calc.
- tot\_magnetization= (if you know for sure. e.g. 0 for antiferromagnetic)  
or can leave it unconstrained to be determined in scf cycle
- starting\_magnetization(i): allowed values between -1 and 1

Should specify non zero starting\_magnetization(i) for at least one species or you will probably get non-magnetic solution

# Input Parameters in “&System”

---

- `ecutwfc`: see the suggested minimum cutoff in the pseudopotential file
- `ecutrho` ( $\sim 4-12 * \text{ecutrho}$ )
- In Rydberg energy units ( $1 \text{ Ry} = 13.6 \text{ eV}$ )

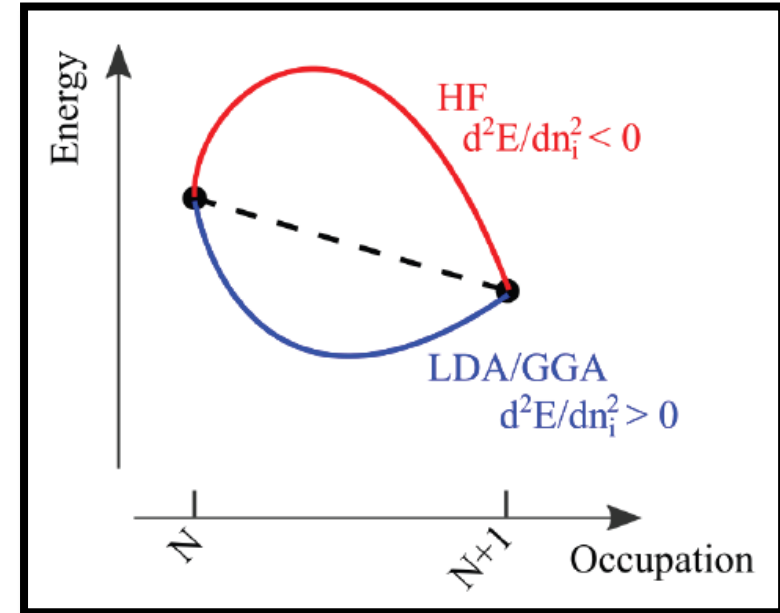
Convergence tests:

typical convergence criterion for the total energy ( $\sim 5 \text{ meV/ atom}$ )

Perform the convergence test for the smallest system possible (primitive cell). Then use `ecutwfc` and `ecutrho` for larger systems.

# Input Parameters in “&System”

- `lda_plus_u = .TRUE.`
- `hubbard_u(i) =` (in eV)
- Koopman's theorem:  
Fractional occupation should be linear
- The perfect U should achieve this linearity



- Note that: you should optimize your cell to a new lattice constant when you add U

# Input Parameters in “&System”

---

- Occupations = ‘fixed’ (for semiconductors and insulators with gap)
- Occupations = ‘smearing’ (for metals or if you have point defects)
- Smearing = ‘Gaussian’ or ‘mv’ (for metals use mv)
- Degauss = value of broadening ( $\sim 0.05$  Ry for metals)
- The smaller , the better



# Input Parameters in “&ELECTRONS”

---

- Can leave it empty and stick to default values while learning
- conv\_thr: Convergence threshold for self-consistency (default is 1.0d-6)
- Mixing beta: mixing factor for self-consistency (default is 0.7)  
may use 0.5 or 0.3 if self-consistency is not achieved after 100 iterations

***&ELECTRONS***

conv\_thr = 1.0d-9

/

# Input Parameters in “&IONS”

---

- Must include it if calculation = ‘relax’ or ‘vc-relax’
- Can leave it empty and stick to default values

**&CELL**

ion\_dynamics = 'bfgs', !default

/

# Input Parameters in “&CELL”

---

- Must include it if calculation= ‘vc-relax’
- It will be ignored if calculation= ‘scf’ or ‘relax’

***&CELL***

cell\_dynamics = 'bfgs' ,     !default

cell\_dofree = 'all',         !default

/

# Cards

---

- Can be in any order

*ATOMIC\_SPECIES*

*ATOMIC\_POSITIONS*

*CELL\_PARAMETERS*

*K\_POINTS*

# ATOMIC\_SPECIES

---

- Must have number of lines = ntyp
- You can choose any name for an atomic species
- Label atoms of interest  
**(to track them or control their magnetization)**
- Use SSSP library (very well tested except for actinides)
- For actinides use pseudopotentials in QE library.

## *ATOMIC\_SPECIES*

Fe1 55.845 Fe.pbe-spn-rrkjus\_psl.0.2.1.UPF

Fe2 55.845 Fe.pbe-spn-rrkjus\_psl.0.2.1.UPF

O 15.999 O.pbe-n-rrkjus\_psl.0.1.UPF

# CELL\_PARAMETERS

- Options: 'bohr' or 'angstrom'
- These are the 3 cell vectors that define your system
- These values can be optimized automatically through "vc-relax"
- Or manually (for cubic structures) by making a set of "scf" calculations varying lattice parameter
- Periodicity will be applied to this cell

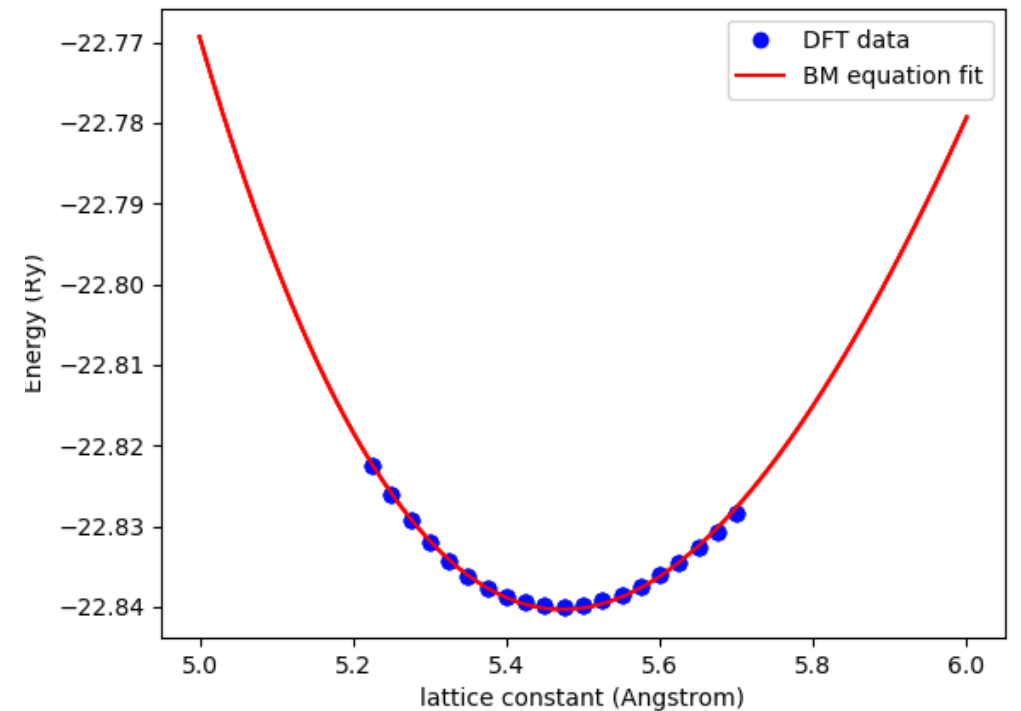
<i>CELL_PARAMETERS</i>	<i>angstrom</i>	
<i>5.47000000</i>	<i>0.00000000</i>	<i>0.00000000</i>
<i>0.00000000</i>	<i>5.47000000</i>	<i>0.00000000</i>
<i>0.00000000</i>	<i>0.00000000</i>	<i>5.47000000</i>

<i>CELL_PARAMETERS</i>	<i>angstrom</i>	
<i>5.439039</i>	<i>0.000000</i>	<i>0.000000</i>
<i>3.097504</i>	<i>4.470863</i>	<i>0.000000</i>
<i>3.097504</i>	<i>1.622263</i>	<i>4.166159</i>

# CELL\_PARAMETERS

---

- Equilibrium lattice constant has the lowest energy
- Also, can calculate theoretical bulk modulus, if you fit the data to a quadratic equation



# ATOMIC\_POSITIONS

- Options: 'bohr', 'angstrom', 'crystal'
- Recommended: **crystal**  
(use fractional coordinates)  
relative coordinates to lattice vectors  
(defined in CELL\_PARAMETERS)
- Must have number of lines = nat
- Keep in mind that **periodic boundary condition** is applied automatically
- So, don't add atoms more than you should  
or they might overlap  
for example, primitive BCC: only 2 atoms

<i>ATOMIC_POSITIONS</i>		<i>crystal</i>	
Fe1	0.144983	0.144983	0.144984
Fe1	0.855016	0.855016	0.855016
Fe2	0.355016	0.355016	0.355016
Fe2	0.644983	0.644983	0.644982
O	0.749999	0.444610	0.055389
O	0.944610	0.249999	0.555389
O	0.444610	0.055389	0.750000
O	0.249999	0.555389	0.944610
O	0.055389	0.749999	0.444610
O	0.555389	0.944610	0.249999



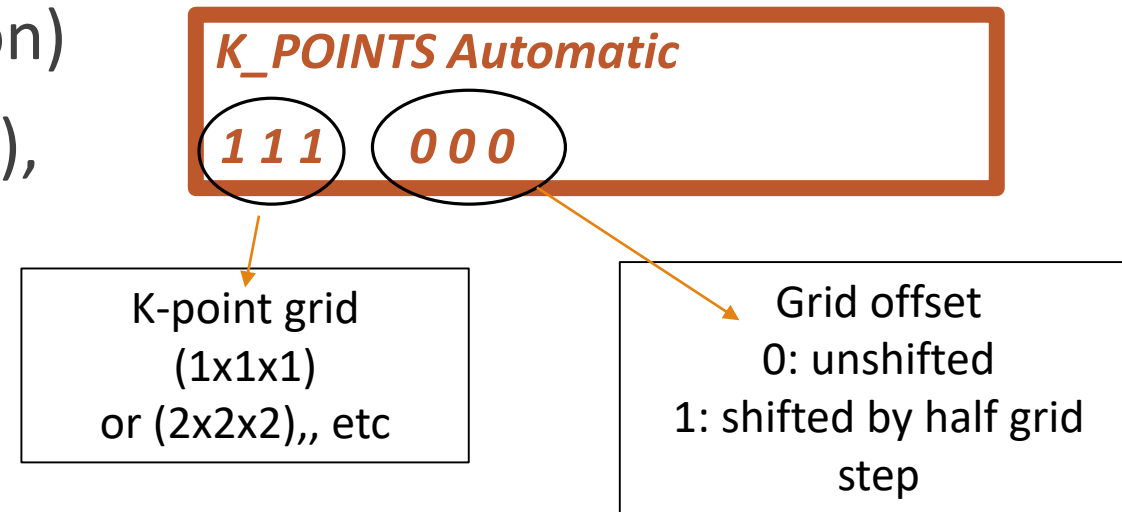
# Using Vesta

---

- Very useful in duplicating primitive cells to generate supercells of any size.
- Export atomic positions in “.vasp” format
- Can import structures from [crystallography.net](http://crystallography.net) in “.CIF” format

# K\_POINTS (reciprocal space)

- Dependent on cell size (inverse relation)
- For very large supercells (> 100 atoms), may use only 1 k-point (gamma point)



For smaller super cells, we need convergence tests

- Options: 'automatic' generates grid using MP scheme (recommended)  
'tpiba' read k-points in Cartesian coordinate units of  $2\pi/a$

# Output

---

To get lines with total energy: `grep ! qe_output_file`

To get lines with pressure or stresses: `grep kbar qe_output_file`

Stresses are calculated automatically in “vc-relax”

Forces are calculated automatically in “relax”

Use dos.x to plot density of states

Use pp.x to extract plottable charge density files