Propriedades Quânticas de Nanomateriais utilizando a Teoria do Funcional Densidade (DFT)

Pedro Venezuela

Marcio Costa

Instituto de Física
Universidade Federal Fluminense

Goals

Introduce the use a DFT code

DFT Code

Which DFT code will be used?

Quantum Espresso (QE)

https://www.quantum-espresso.org/

There are several DFT codes. Why QE?

- Open source
- Plane wave
- Good support
- Online resources

Linux Installation

Where are we going to run QE?

Linux machine

Which distribution?

Ubuntu

How to?

- Full Linux machine
- Dual boot machine
- Virtual machine
- Bootable USB

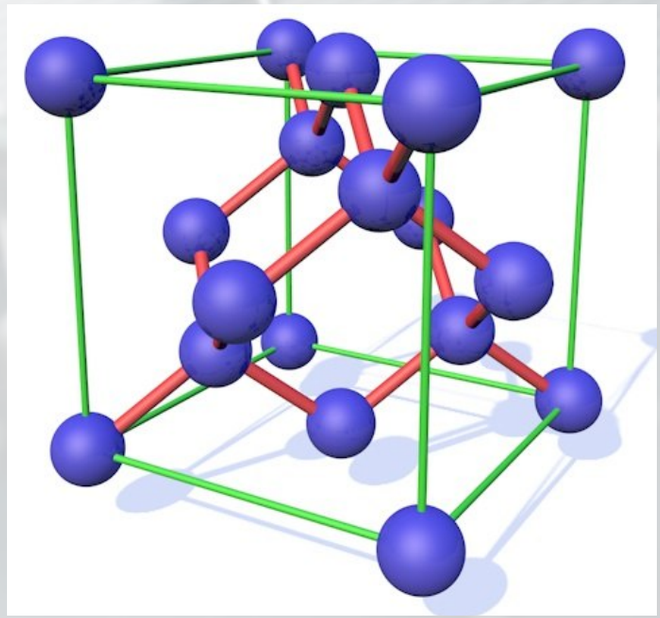
Tutorials

Tutorials to be performed during the course

Practical Part

Silicon

- Bulk SCF (initial convergency tests)
- Total and projected density of states
- Bulk band structure
- FCC lattice parameter (convergency tests)
- FCC bulk modulus
- FCC lattice parameter - VC-relax



Practical Part

Iron

- Non spin polarized band structure (1 atom unit cell)
- Spin polarized band structure (1 atom unit cell)
- Total and projected density of states (SP and Non SP)

Practical Part

Graphene

- Band Structure
- Total and projected density of states
- Carbon phase diagram: Diamond X Honeycomb
- Phonons

Practical Part

Graphite

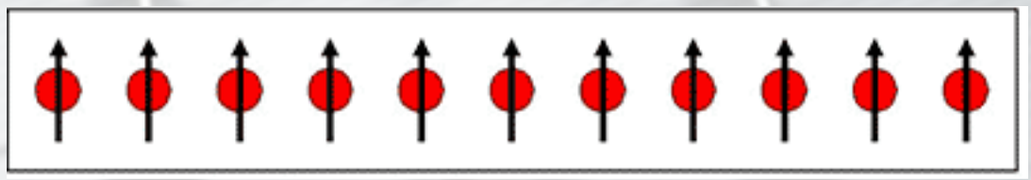
- Inter-planar distance
  - LDA
  - GGA
  - LDA + vdW correction
  - GGA + vdW correction

Practical Part

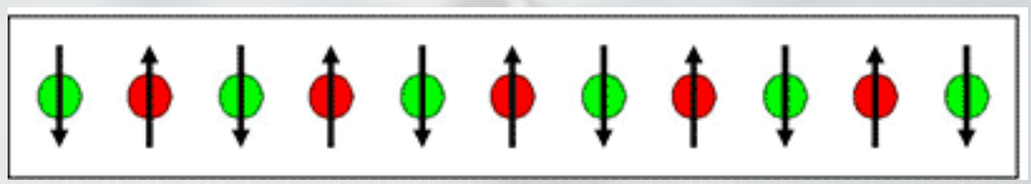
2D Magnetic Material - FeSe

- Band structure
- DOS and PDOS
- Magnetic ground state - AFM x FM

Ferromagnetic - FM



Antiferromagnetic - AFM



- Spin polarized density

Input Description

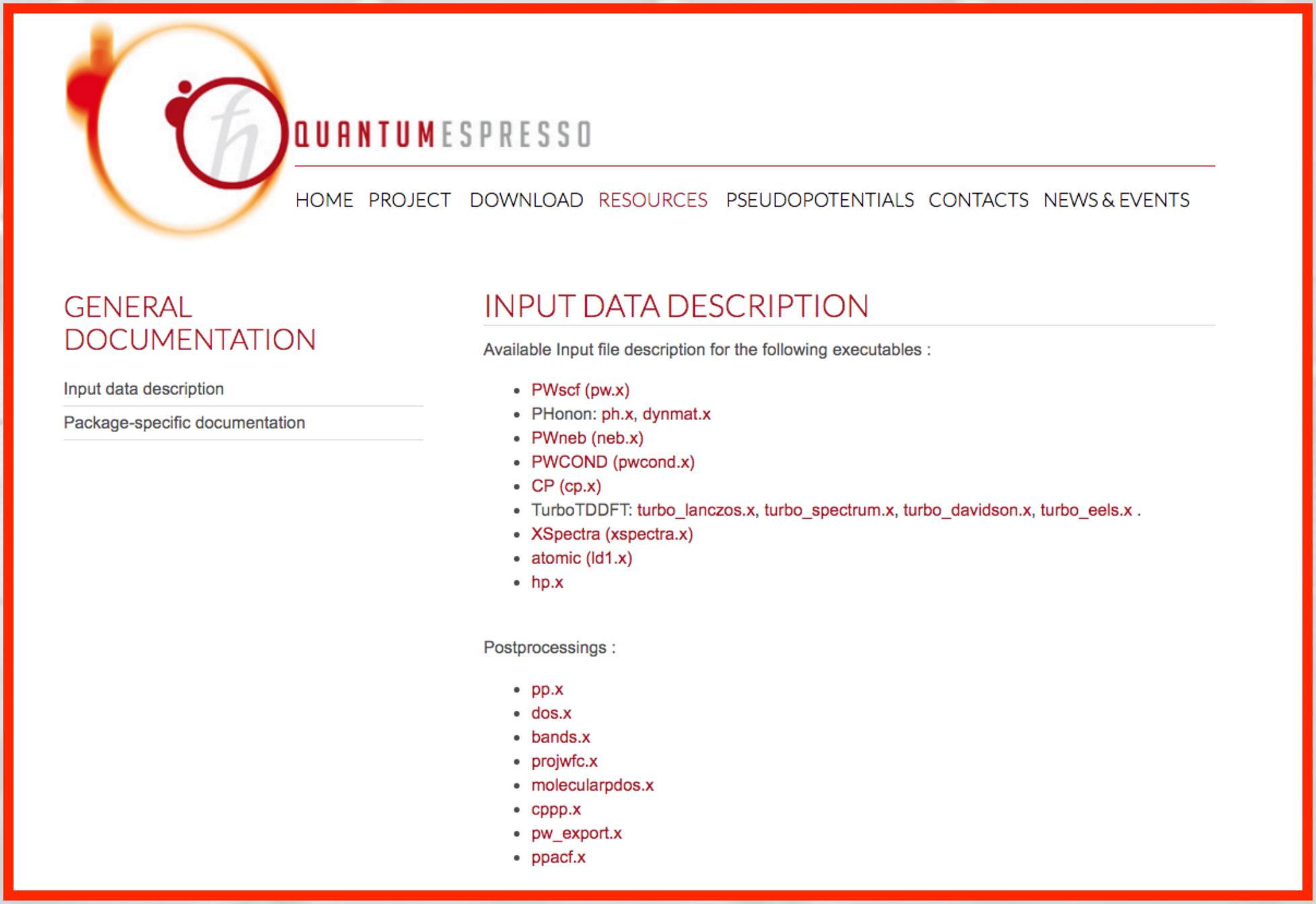
Basic QE input

Si Bulk

```
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/mcosta/dft_online/pseudos',
   outdir='./'
/
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =18.0,
   ecutrho = 72.0,
 /
 &electrons
   diagonalization='david'
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
```

Si Bulk

https://www.quantum-espresso.org/resources/users-manual/input-data-description



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```

Si Bulk

```
&control
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```

calculation type

calculation	CHARACTER
Default:	'scf'

A string describing the task to be performed. Options are:

```
'scf'

'nscf'

'bands'

'relax'

'md'

'vc-relax'

'vc-md'
```

(vc = variable-cell).

```
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ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
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 4 4 4 0 0 0
```

starting mode

Si Bulk

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ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
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```

system name

Si Bulk

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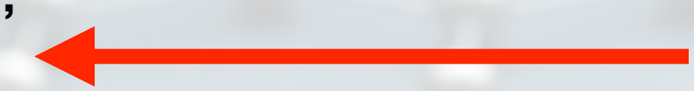

calculates stress tensor

Si Bulk

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 Si 0.25 0.25 0.25
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 4 4 4 0 0 0
```

calculates forces

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```
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ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
```

pseudo potential path

Si Bulk

```
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ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
```

output path

Si Bulk

```
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   p
   t
   t
   p
   c
/
&s
   i
   c
   n
   n
   e
   e
/
&e
   c
   n
   n
   c
/
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
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 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
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 4 4 4 0 0 0
```

&CONTROL

calculation | title | verbosity | restart_mode | wf_collect | nstep | iprint | tstress | tprnfor | dt | outdir | wfcdir | prefix | lkpoint_dir | max_seconds | etot_conv_thr | forc_conv_thr | disk_io | pseudo_dir | tefield | dipfield | lelfield | nberrycyc | lorbm | lberry | gdir | nppstr | lfcpopt | gate

&SYSTEM

ibrav | celldm | A | B | C | cosAB | cosAC | cosBC | nat | ntyp | nbnd | tot_charge | starting_charge | tot_magnetization | starting_magnetization | ecutwfc | ecutrho | ecutfock | nr1 | nr2 | nr3 | nr1s | nr2s | nr3s | nosym | nosym_evc | noinv | no_t_rev | force_symmorphic | use_all_frac | occupations | one_atom_occupations | starting_spin_angle | degauss | smearing | nspin | noncolin | ecfixed | qcutz | q2sigma | input_dft | exx_fraction | screening_parameter | exxdiv_treatment | x_gamma_extrapolation | ecutvcut | nqx1 | nqx2 | nqx3 | localization_thr | lda_plus_u | lda_plus_u_kind | Hubbard_U | Hubbard_J0 | Hubbard_alpha | Hubbard_beta | Hubbard_J | starting_ns_eigenvalue | U_projection_type | edir | emaxpos | eopreg | eamp | angle1 | angle2 | lforcet | constrained_magnetization | fixed_magnetization | lambda | report | lspinorb | assume_isolated | esm_bc | esm_w | esm_efield | esm_nfit | fcp_mu | vdw_corr | london | london_s6 | london_c6 | london_rvdw | london_rcut | dftd3_version | dftd3_threebody | ts_vdw_econv_thr | ts_vdw_isolated | xdm | xdm_a1 | xdm_a2 | space_group | uniqueb | origin_choice | rhombohedral | zgate | relaxz | block | block_1 | block_2 | block_height

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```

Bravais lattice

Si Bulk

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/
&system
   ibrav=  2,
   celldm(1) =10.20,
```

Bravais lattice

```
ibrav      structure                   celldm(2)-celldm(6)
                                     or: b,c,cosbc,cosac,cosab
  0          free
      crystal axis provided in input: see card CELL_PARAMETERS

  1          cubic P (sc)
      v1 = a(1,0,0),  v2 = a(0,1,0),  v3 = a(0,0,1)

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

  3          cubic I (bcc)
      v1 = (a/2)(1,1,1),  v2 = (a/2)(-1,1,1),  v3 = (a/2)(-1,-1,1)
 -3          cubic I (bcc), more symmetric axis:
      v1 = (a/2)(-1,1,1), v2 = (a/2)(1,-1,1),  v3 = (a/2)(1,1,-1)

  4          Hexagonal and Trigonal P          celldm(3)=c/a
      v1 = a(1,0,0),  v2 = a(-1/2,sqrt(3)/2,0),  v3 = a(0,0,c/a)
```

K_POINTS automatic
4 4 4 0 0 0

Si Bulk

```
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```

lattice parameter (Bohr)

Si Bulk

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 4 4 4 0 0 0
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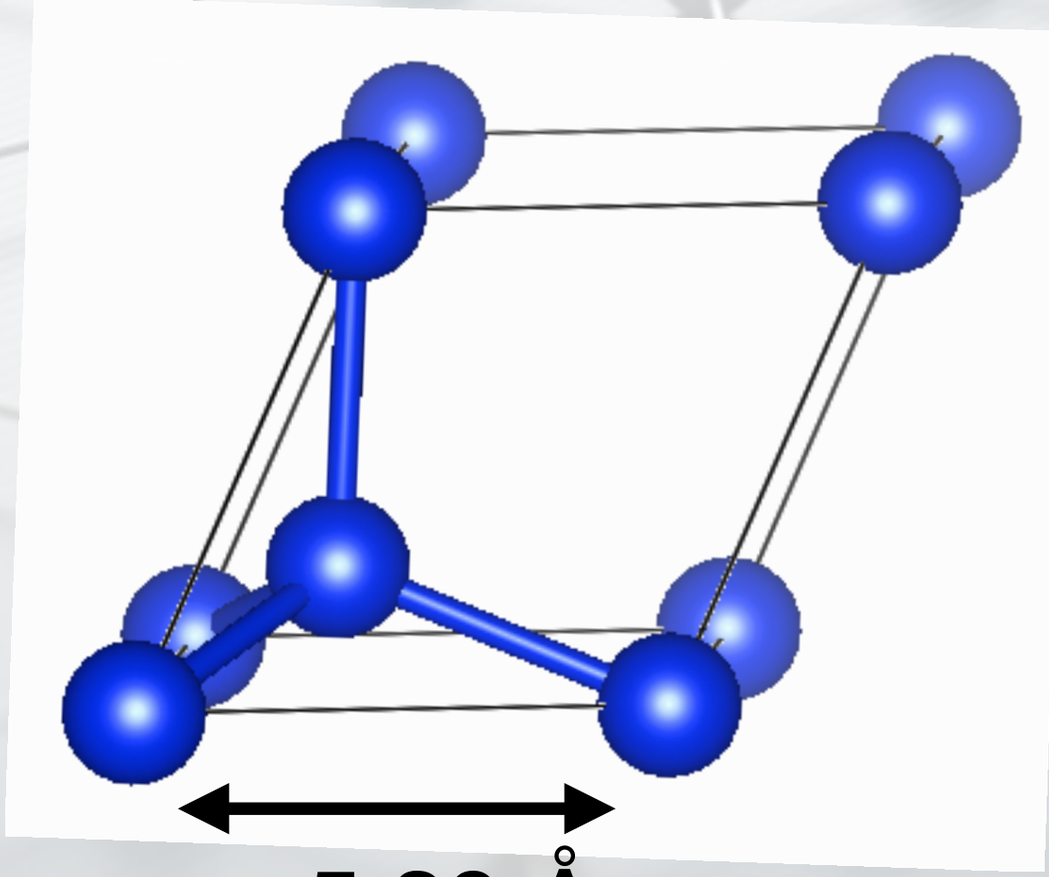
lattice parameter (Bohr)



a = 5.39 Å

Si Bulk

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number of atoms

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```

number of types

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```

wave function cutoff energy

Si Bulk

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 Si 0.25 0.25 0.25
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 4 4 4 0 0 0
```

charge density cutoff energy

Si Bulk

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diagonalization type

Si Bulk

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   tprnfor
   pseudo
   outdir=
/
&system
   ibrav=
   celldm(
   nat= 2,
   ntyp= 1
   ecutwf
   ecutrho
 /
 &electron
   diagona
   mixing_
   mixing_
   conv_th
 /
ATOMIC_
 Si  28.086
ATOMIC_
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
```

diagonalization type

```
'david' :
     Davidson iterative diagonalization with overlap matrix
     (default). Fast, may in some rare cases fail.

'cg' :
     Conjugate-gradient-like band-by-band diagonalization.
     Slower than 'david' but uses less memory and is
     (a little bit) more robust.

'cg-serial', 'david-serial' :
     OBSOLETE, use -ndiag 1 instead.
     The subspace diagonalization in Davidson is performed
     by a fully distributed-memory parallel algorithm on
     4 or more processors, by default. The allocated memory
     scales down with the number of procs. Procs involved
     in diagonalization can be changed with command-line
     option -ndiag N. On multicore CPUs it is often
     convenient to let just one core per CPU to work
     on linear algebra.
```

Si Bulk

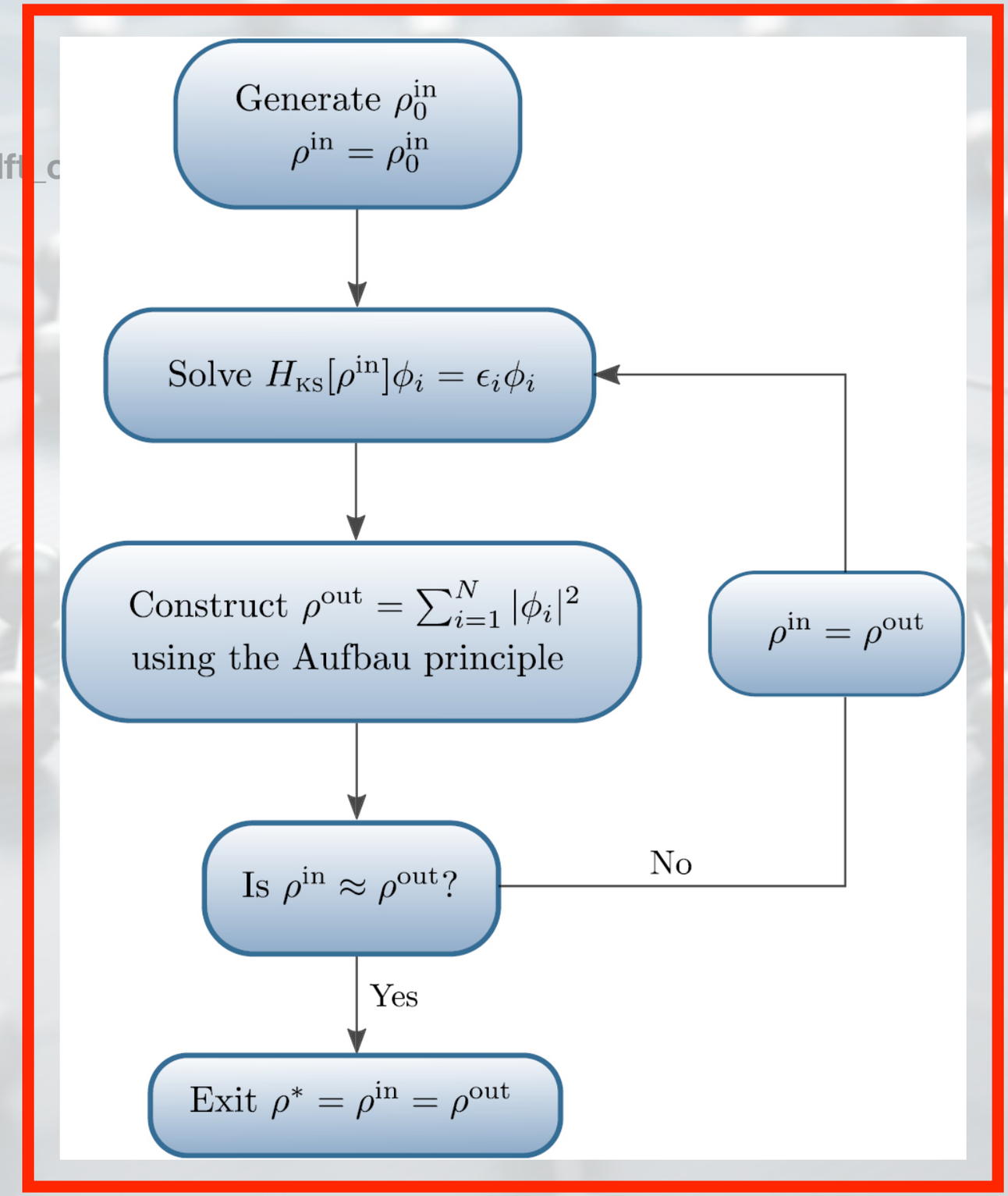
```
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/mcosta/dft_online/pseudos',
   outdir='./'
/
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =18.0,
   ecutrho = 72.0,
 /
 &electrons
   diagonalization='david'
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
```

charge density mixing

Si Bulk

```
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/mcosta/dft_c
   outdir='./'
/
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =18.0,
   ecutrho = 72.0,
 /
 &electrons
   diagonalization='david'
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
```

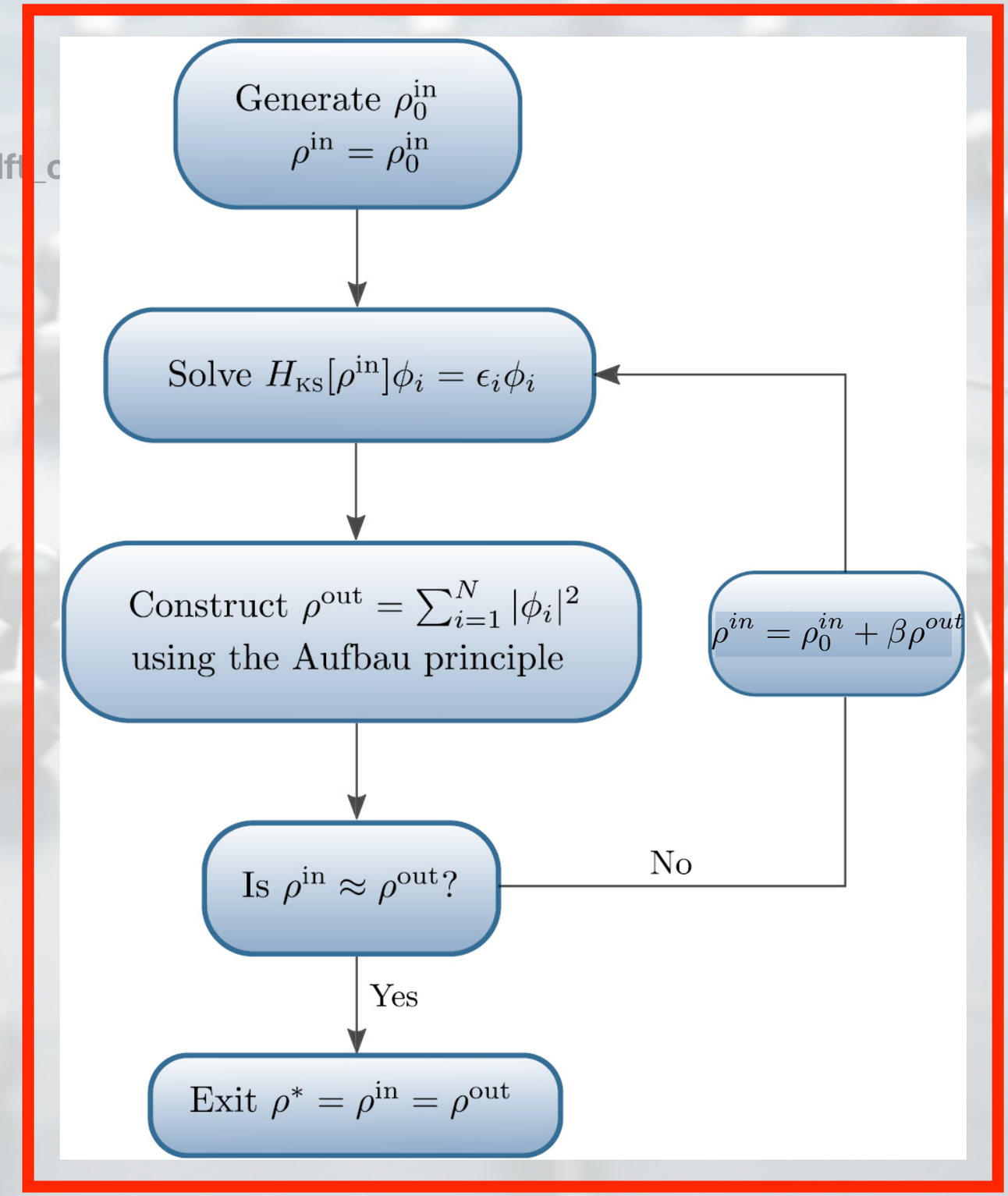
SCF cycle



Si Bulk

```
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/mcosta/dft_c
   outdir='./'
/
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =18.0,
   ecutrho = 72.0,
 /
 &electrons
   diagonalization='david'
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
```

SCF cycle



Si Bulk

```
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/mcosta/dft_online/pseudos',
   outdir='./'
/
&system
   ibrav=  2,
   celldm(1) =10.20
   nat=  2,
   ntyp= 1,
   ecutwfc =18.0,
   ecutrho = 72.0,
 /
 &electrons
   diagonalization=
   mixing_mode = '
   mixing_beta = 0.
   conv_thr =  1.0d-
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
```

charge density mixing

```
'plain'  :
      charge density Broyden mixing

'TF'  :
     as above, with simple Thomas-Fermi screening
     (for highly homogeneous systems)

'local-TF'  :
     as above, with local-density-dependent TF screening
     (for highly inhomogeneous systems)
```

Si Bulk

```
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/mcosta/dft_online/pseudos',
   outdir='./'
/
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =18.0,
   ecutrho = 72.0,
 /
 &electrons
   diagonalization='david'
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
```

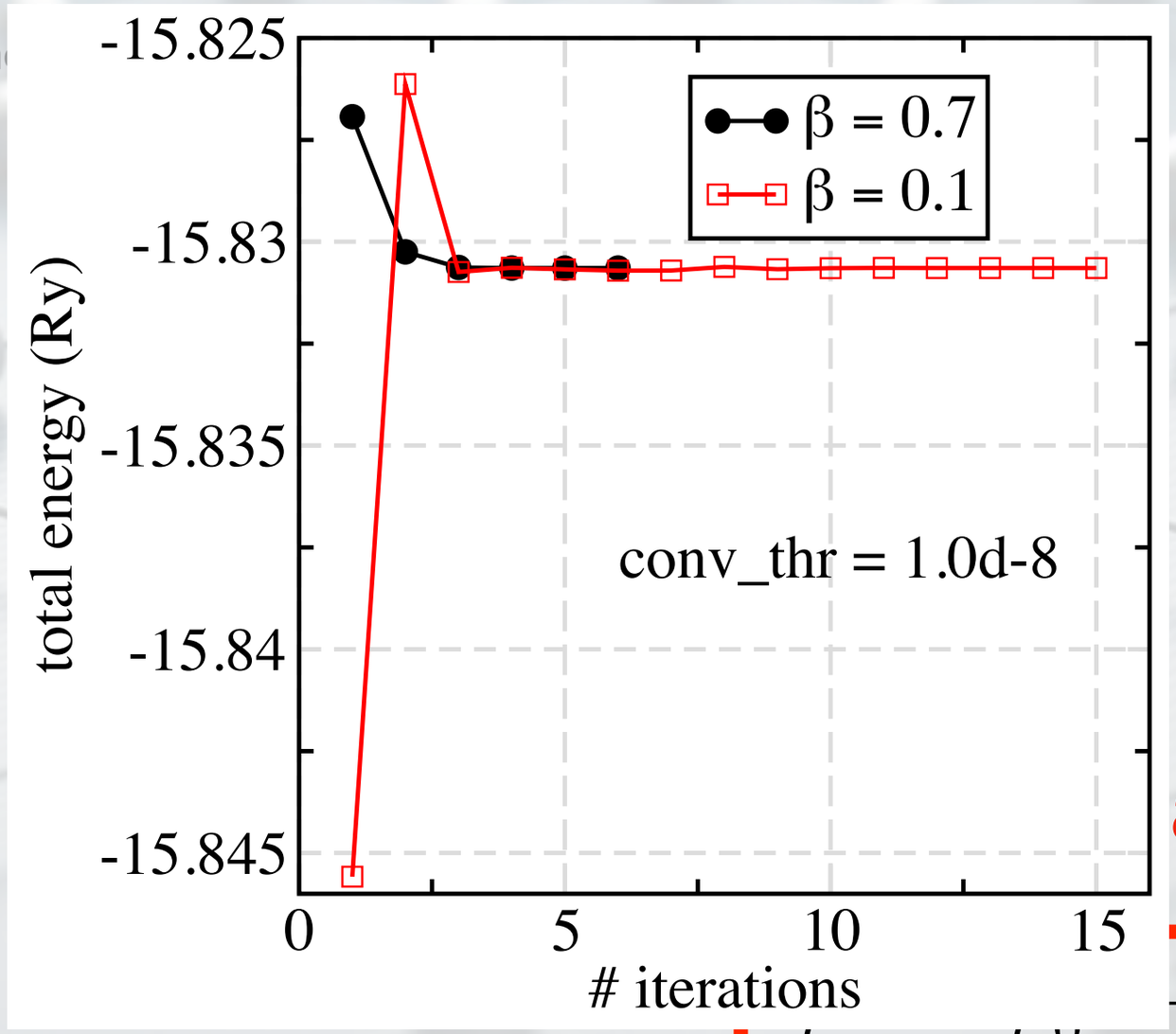
mixing value

$$\rho^{in} = \rho_0^{in} + \beta \rho^{out}$$

Si Bulk

```
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/m
   outdir='./'
/
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =18.0,
   ecutrho = 72.0,
 /
 &electrons
   diagonalization='david'
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
```

mixing value



alue

$$\rho^{new} = \rho^{old} - \beta\rho^{out}$$

Si Bulk

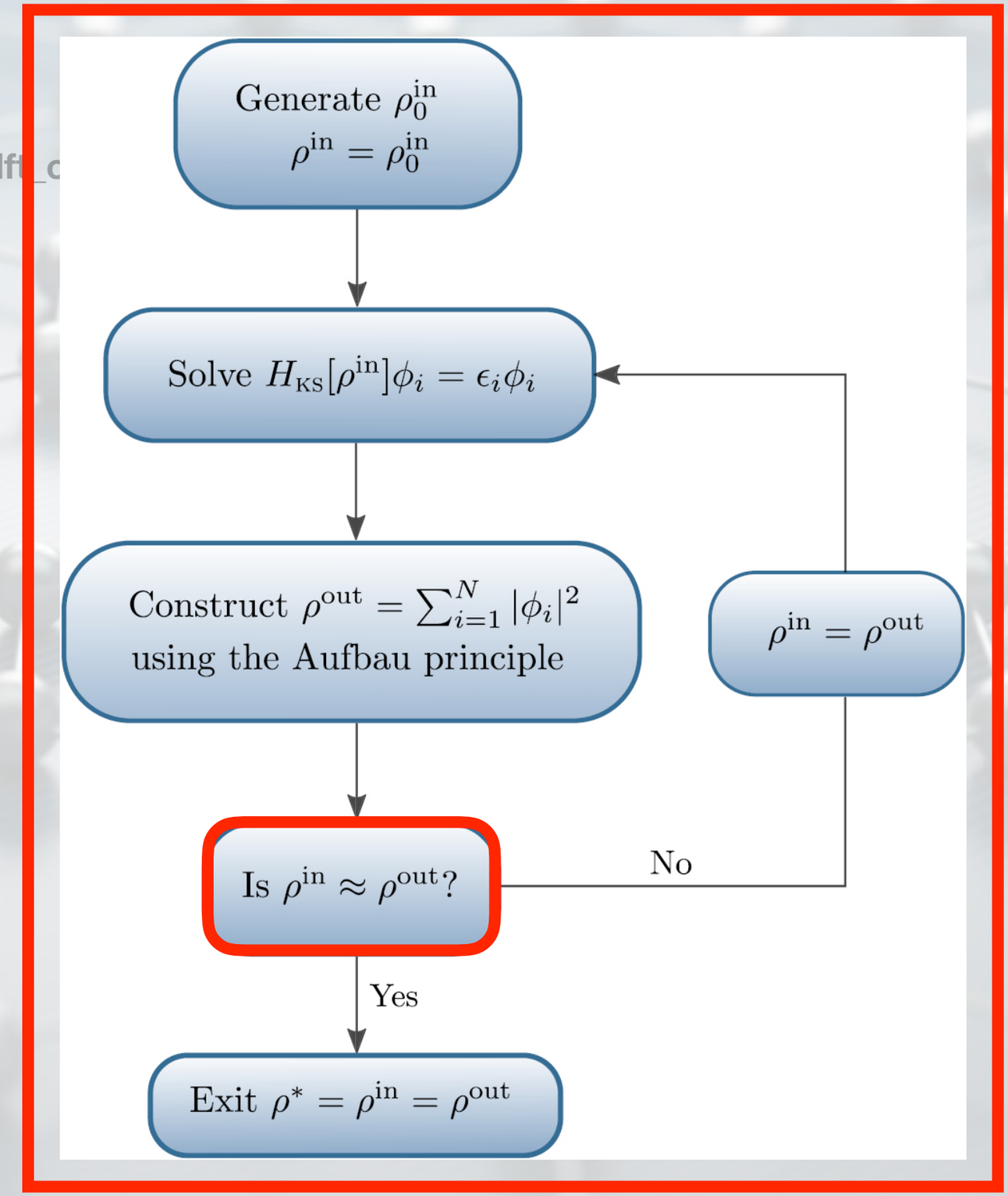
```
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/mcosta/dft_online/pseudos',
   outdir='./'
/
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =18.0,
   ecutrho = 72.0,
 /
 &electrons
   diagonalization='david'
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
```

charge convergency threshold

Si Bulk

charge convergency threshold

```
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/mcosta/dft_c
   outdir='./'
/
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =18.0,
   ecutrho = 72.0,
 /
 &electrons
   diagonalization='david'
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
```



Si Bulk

```
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/mcosta/dft_online/pseudos',
   outdir='./'
/
&system
   ibrav=  2,
   celldm(1) =10.20,
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   ecutwfc =18.0,
   ecutrho = 72.0,
 /
 &electrons
   diagonalization='david'
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
```

Atom , charge , pseudo potential

Si Bulk

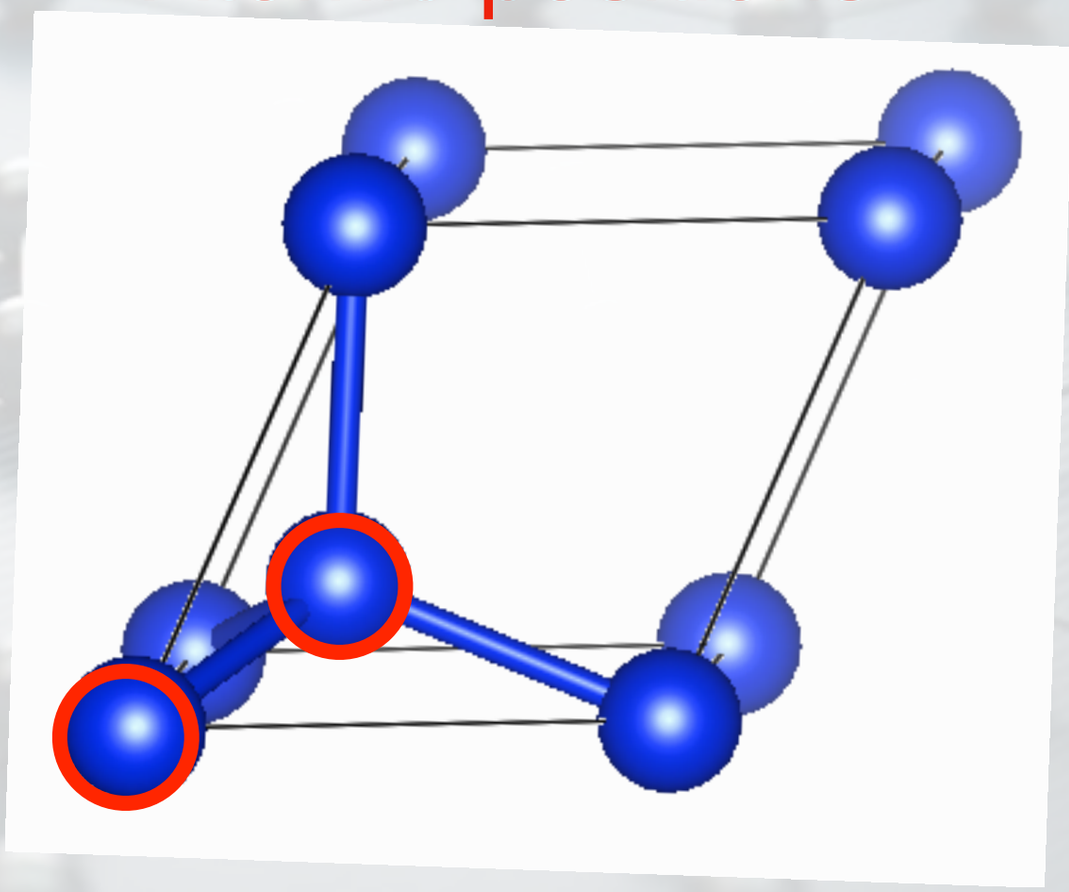
```
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/mcosta/dft_online/pseudos',
   outdir='./'
/
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =18.0,
   ecutrho = 72.0,
 /
 &electrons
   diagonalization='david'
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
```

Atomic positions

Si Bulk

```
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/mcosta/dft_online/pseudos',
   outdir='./'
/
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =18.0,
   ecutrho = 72.0,
 /
 &electrons
   diagonalization='david'
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
```

Atomic positions



Si Bulk

```
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/mcosta/dft_online/pseudos',
   outdir='./'
/
&system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =18.0,
   ecutrho = 72.0,
 /
 &electrons
   diagonalization='david'
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
```

reciprocal space sampling

Wave function cutoff energy

```
#!/bin/bash

dir_files="ecutwfc-in-out-files"

for ecutwfc in `seq 10 5 50`; do

cat > si.scf.$ecutwfc.in <<EOF
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/mcosta/dft_online/pseudos',
   outdir='./'
 /
 &system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =$ecutwfc,
 /
 &electrons
   diagonalization='david'
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
EOF

pw.x < si.scf.$ecutwfc.in > si.scf.$ecutwfc.out

total_energy=`grep ! si.scf.$ecutwfc.out | awk '{print $5}'
echo $ecutwfc $total_energy >> ecutwfcXtotal_energy.dat
mv si.scf.$ecutwfc.in si.scf.$ecutwfc.out $dir_files

done
```

Wave functional cutoff energy

Wave function cutoff energy

```
#!/bin/bash

dir_files="ecutwfc-in-out-files"

for ecutwfc in `seq 10 5 50`; do

cat > si.scf.$ecutwfc.in <<EOF
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/mcosta/dft_online/pseudos',
   outdir='./'
 /
 &system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =$ecutwfc,
 /
 &electrons
   diagonalization='david'
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
EOF

pw.x < si.scf.$ecutwfc.in > si.scf.$ecutwfc.out

total_energy=`grep ! si.scf.$ecutwfc.out | awk '{print $5}'
echo $ecutwfc $total_energy >> ecutwfcXtotal_energy.dat
mv si.scf.$ecutwfc.in si.scf.$ecutwfc.out $dir_files

done
```

Loop from 10 - 50 Ryd

Wave function cutoff energy

```
#!/bin/bash

dir_files="ecutwfc-in-out-files"

for ecutwfc in `seq 10 5 50`; do

cat > si.scf.$ecutwfc.in <<EOF
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/mcosta/dft_online/pseudos',
   outdir='./'
 /
 &system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =$ecutwfc,
 /
 &electrons
   diagonalization='david'
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
EOF

pw.x < si.scf.$ecutwfc.in > si.scf.$ecutwfc.out

total_energy=`grep ! si.scf.$ecutwfc.out | awk '{print $5}'
echo $ecutwfc $total_energy >> ecutwfcXtotal_energy.dat
mv si.scf.$ecutwfc.in si.scf.$ecutwfc.out $dir_files

done
```

Executing pw.x

Wave function cutoff energy

```
#!/bin/bash

dir_files="ecutwfc-in-out-files"

for ecutwfc in `seq 10 5 50`; do

cat > si.scf.$ecutwfc.in <<EOF
&control
   calculation = 'scf'
   restart_mode='from_scratch',
   prefix='silicon',
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = '/home/mcosta/dft_online/pseudos',
   outdir='./'
 /
 &system
   ibrav=  2,
   celldm(1) =10.20,
   nat=  2,
   ntyp= 1,
   ecutwfc =$ecutwfc,
 /
 &electrons
   diagonalization='david'
   mixing_mode = 'plain'
   mixing_beta = 0.7
   conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
EOF

pw.x < si.scf.$ecutwfc.in > si.scf.$ecutwfc.out

total_energy=`grep ! si.scf.$ecutwfc.out | awk '{print $5}'
echo $ecutwfc $total_energy >> ecutwfcXtotal_energy.dat
mv si.scf.$ecutwfc.in si.scf.$ecutwfc.out $dir_files

done
```

Getting the total energy form the output

Wave function cutoff energy

```
#!/bin/bash

dir_files="ecutwfc-in-out-files"

for ecutwfc in `seq 10 5 50`; do

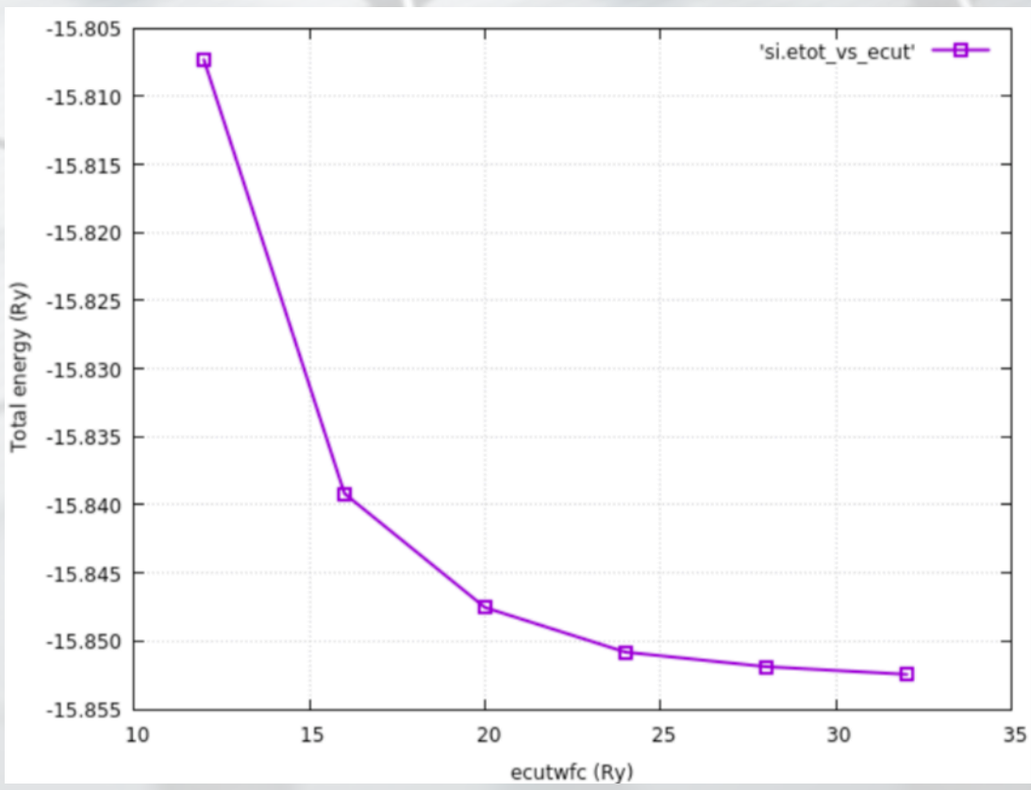
cat > si.scf.$ecutwfc.in <<EOF
&control
    calculation = 'scf'
    restart_mode='from_scratch',
    prefix='silicon',
    tstress = .true.
    tprnfor = .true.
    pseudo_dir = '/home/mcosta/dft_online/pseudos',
    outdir='./'
 /
 &system
    ibrav=  2,
    celldm(1) =10.20,
    nat=  2,
    ntyp= 1,
    ecutwfc =$ecutwfc,
 /
 &electrons
    diagonalization='david'
    mixing_mode = 'plain'
    mixing_beta = 0.7
    conv_thr =  1.0d-8
 /
ATOMIC_SPECIES
 Si  28.086  Si.pz-vbc.UPF
ATOMIC_POSITIONS alat
 Si 0.00 0.00 0.00
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4 0 0 0
EOF

pw.x < si.scf.$ecutwfc.in > si.scf.$ecutwfc.out

total_energy=`grep ! si.scf.$ecutwfc.out | awk '{print $5}'
echo $ecutwfc $total_energy >> ecutwfcXtotal_energy.dat
mv si.scf.$ecutwfc.in si.scf.$ecutwfc.out $dir_files

done
```

ecutwfc X total energy



Wave function cutoff energy

Different problems require different parameters

- Phase diagrams
- Adsorption energy
- Magnetic ground state
- others

Wave function cutoff energy

Different problems require different parameters

- Phase diagrams
- Adsorption energy
- Magnetic ground state
- others