Quantum Espresso Tutorial

Hands-on Session #1

First steps with QE: total energy and relaxations

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

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06.02.13

PATCHES FOR QUANTUM ESPRESSO V.5.0.2

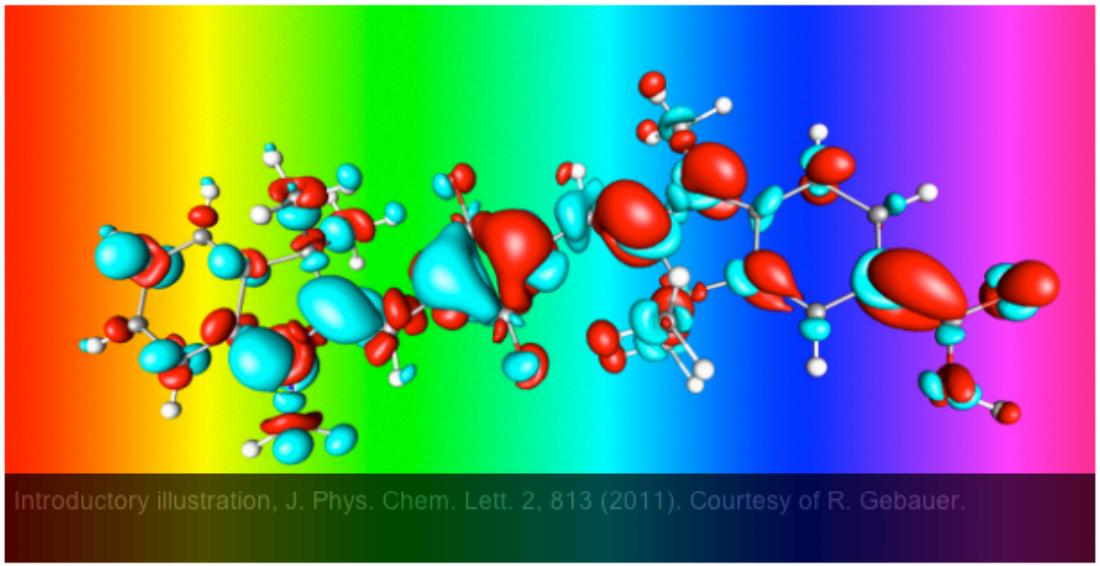
Patches for Quantum ESPRESSO v.5.0.2 (**corrected on May 6**) are available from the download page. Look for Release Name 5.0.3. Instructions **here**.

13.12.12

QUANTUM ESPRESSO EVENTS 2013

Hands-on Tutorial on Electronic Structure Computations, ICTP Trieste, 14-18 January.

Workshop on Computer Programming and Advanced Tools for Scientific Research Work & Quantum ESPRESSO Developer Training, ICTP Trieste, 11-28 March



Introductory illustration, J. Phys. Chem. Lett. 2, 813 (2011). Courtesy of R. Gebauer.

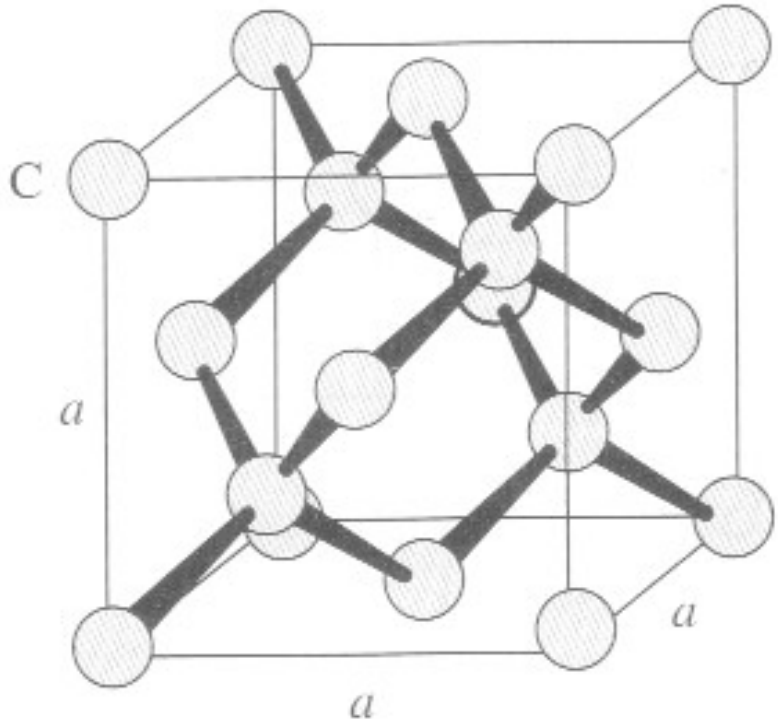
QUANTUM ESPRESSO

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

READ MORE >

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
```



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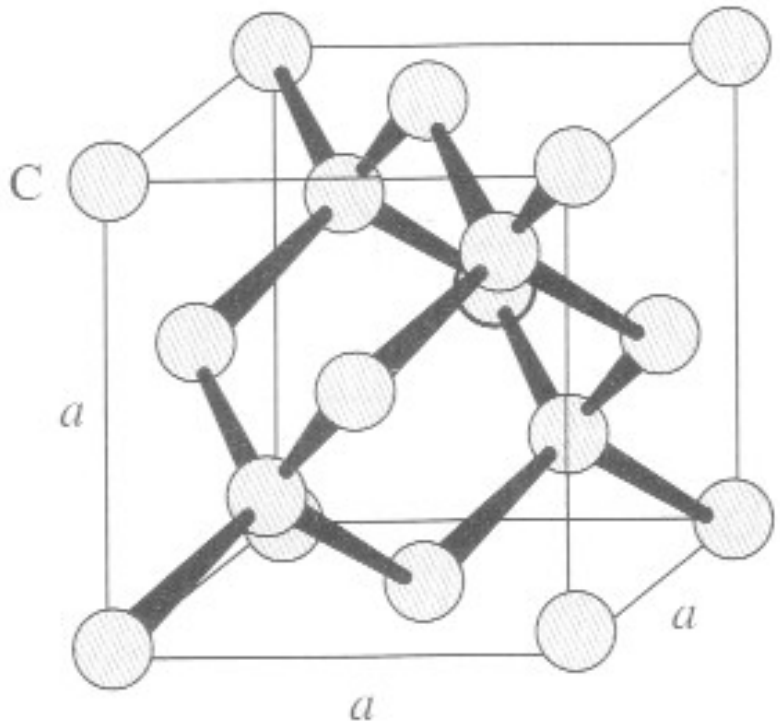
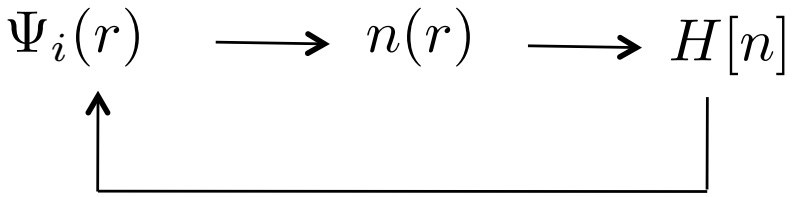
 Si 0.25 0.25 0.25
K_POINTS (automatic)
 6 6 6 1 1 1
```



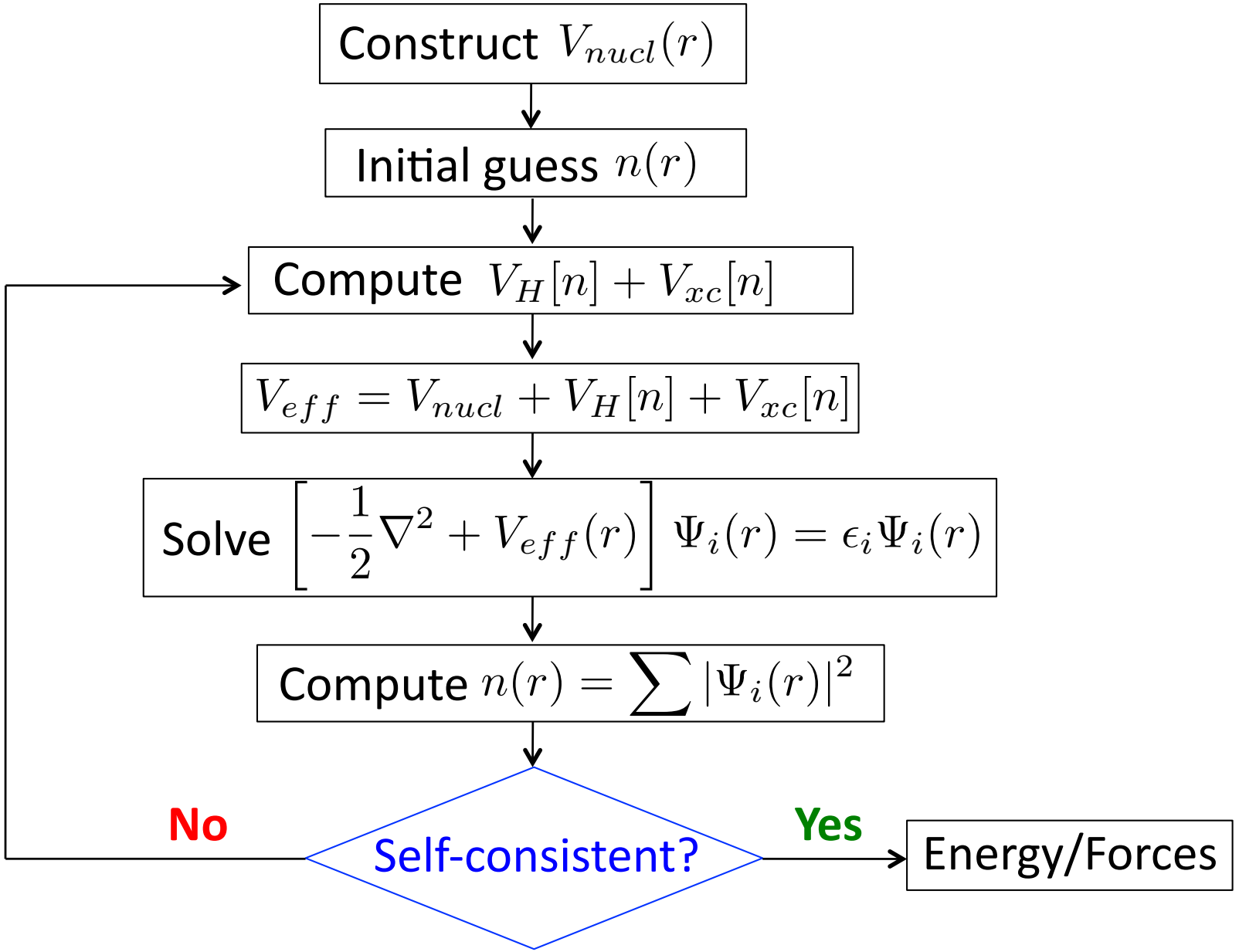
The Kohn-Sham problem

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

SCF:



Iterative solution of KS equations



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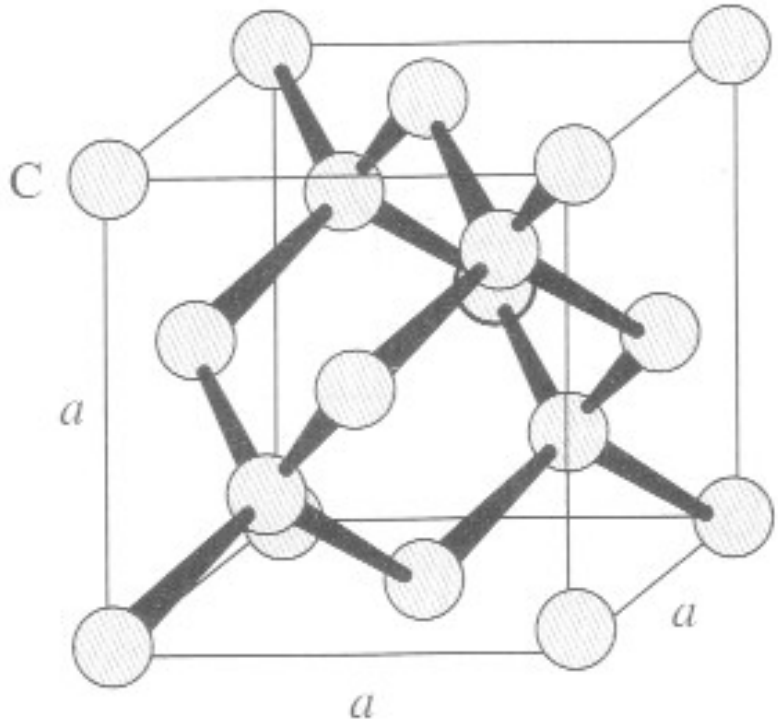
 Si 0.0 0.0 0.0
 Si 0.25 0.25 0.25
K_POINTS (automatic)
 6 6 6 1 1 1
```



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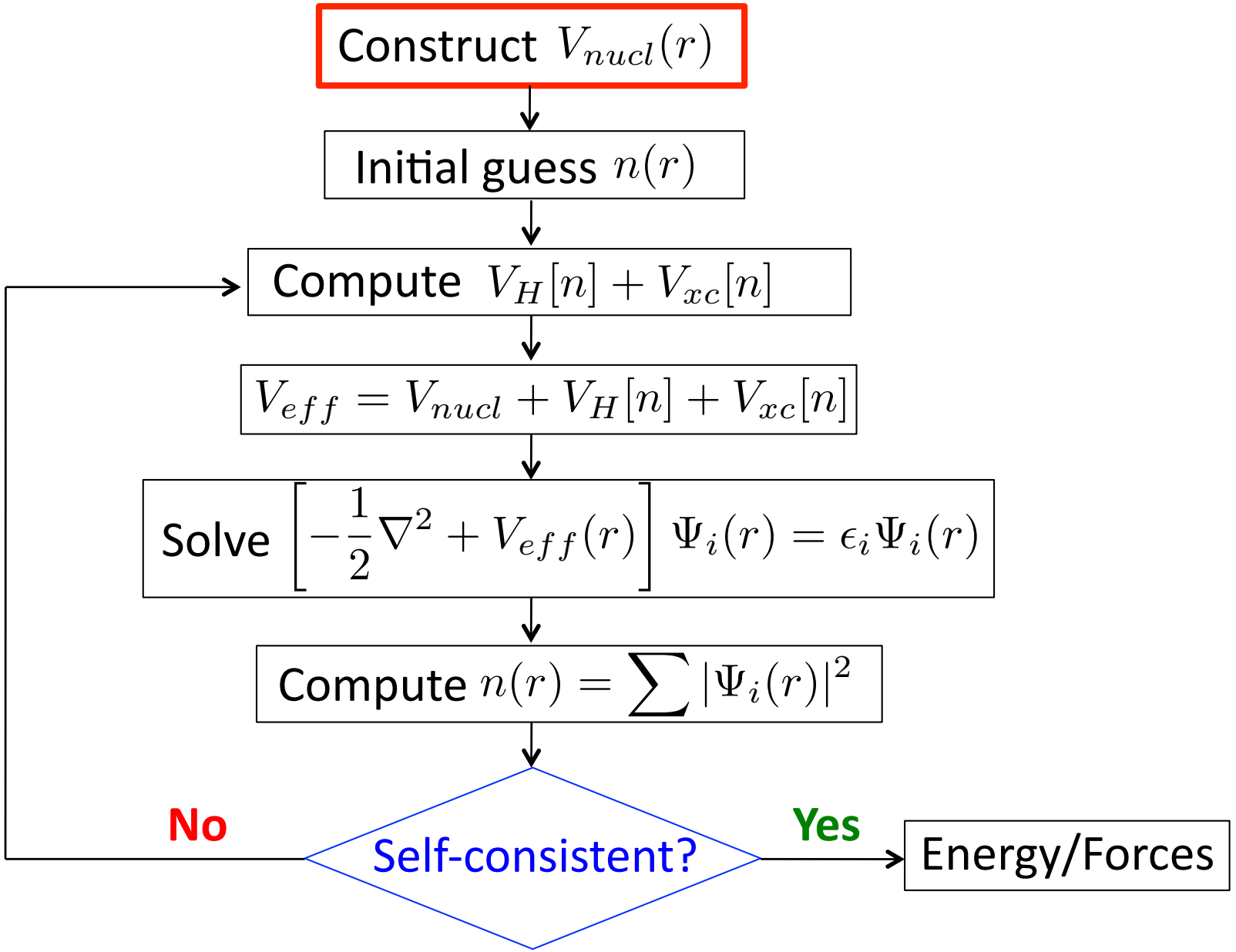
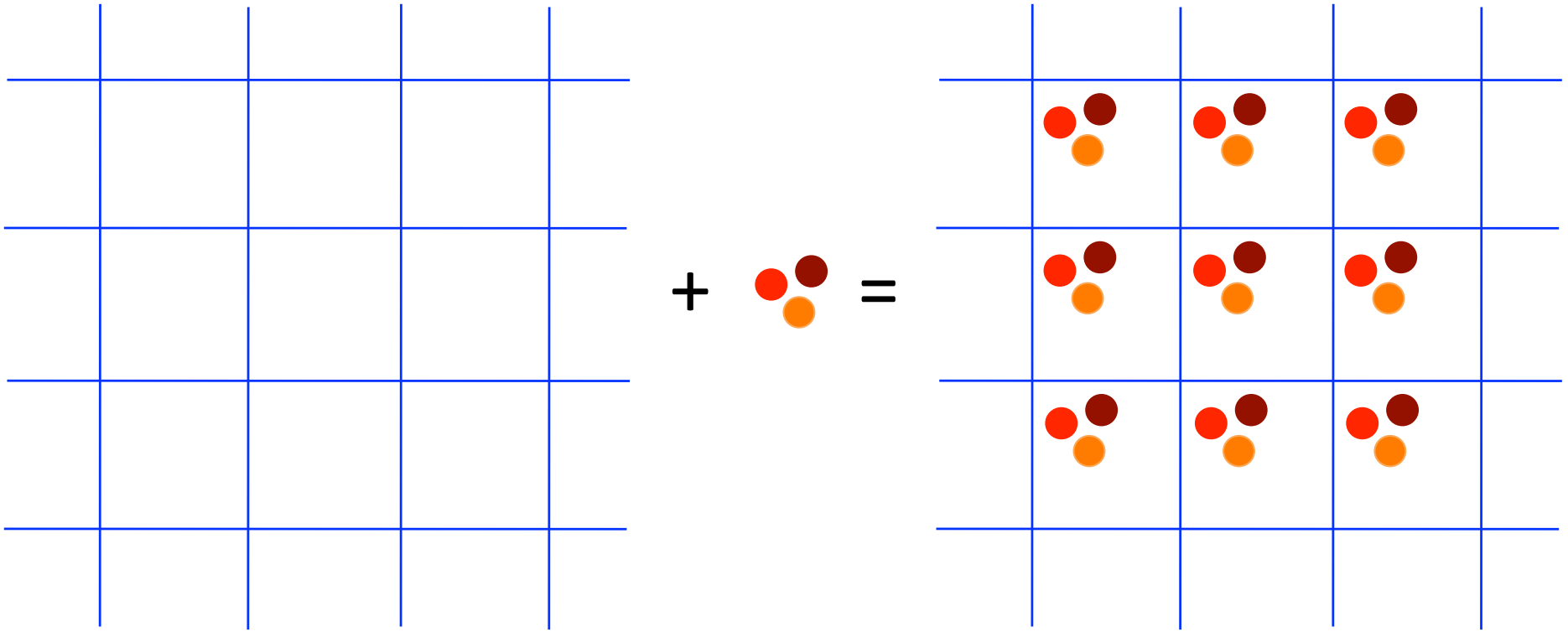
```

Iterative solution of KS equations



Periodic Boundary Conditions

Periodic system: lattice + 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

```
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   calculation = 'scf',
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&system
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 Si 0.0 0.0 0.0
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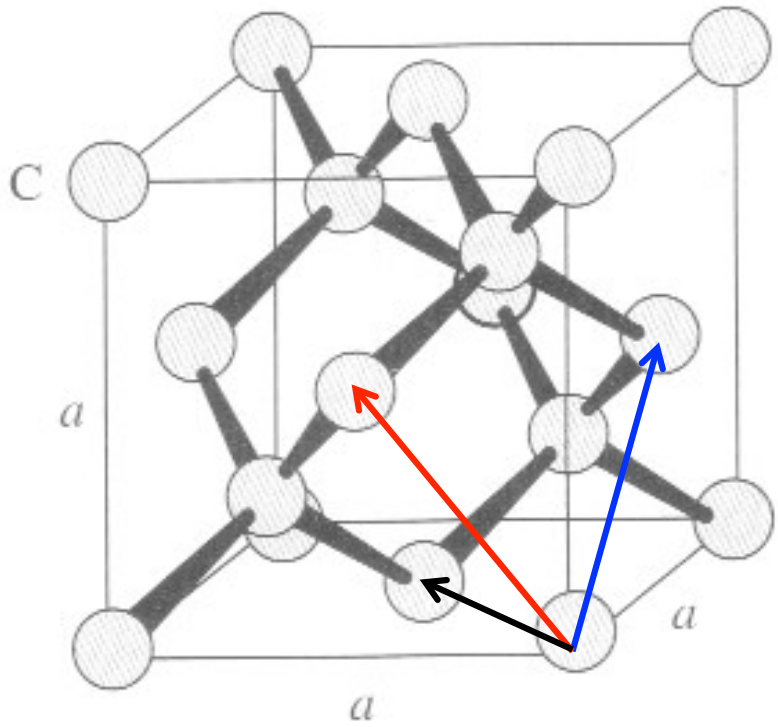

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 Si 0.0 0.0 0.0
 Si 0.25 0.25 0.25
K_POINTS (automatic)
 6 6 6 1 1 1
```

Units: bohr (1 bohr = 0.529177 Å)

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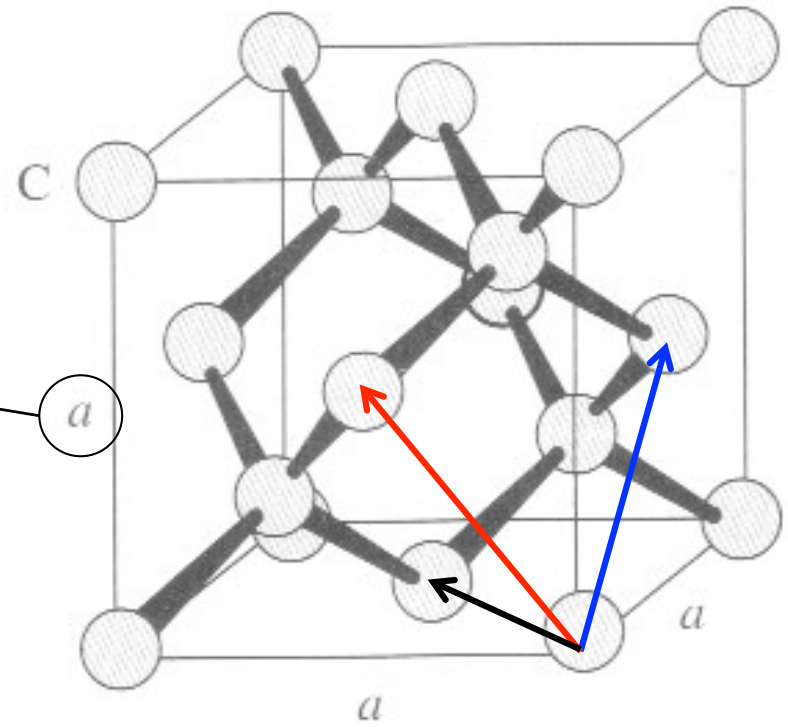

fcc:

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

Structure of QE input file

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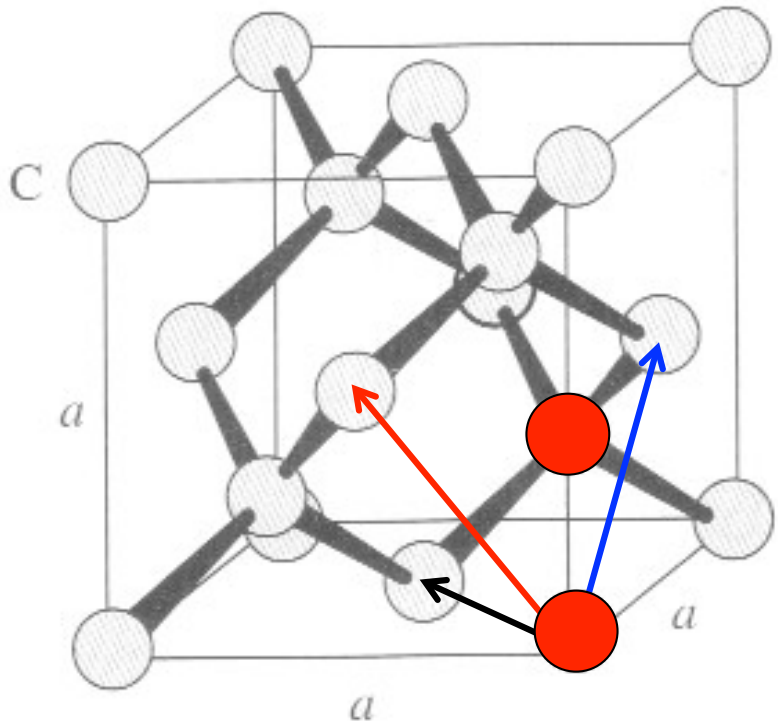

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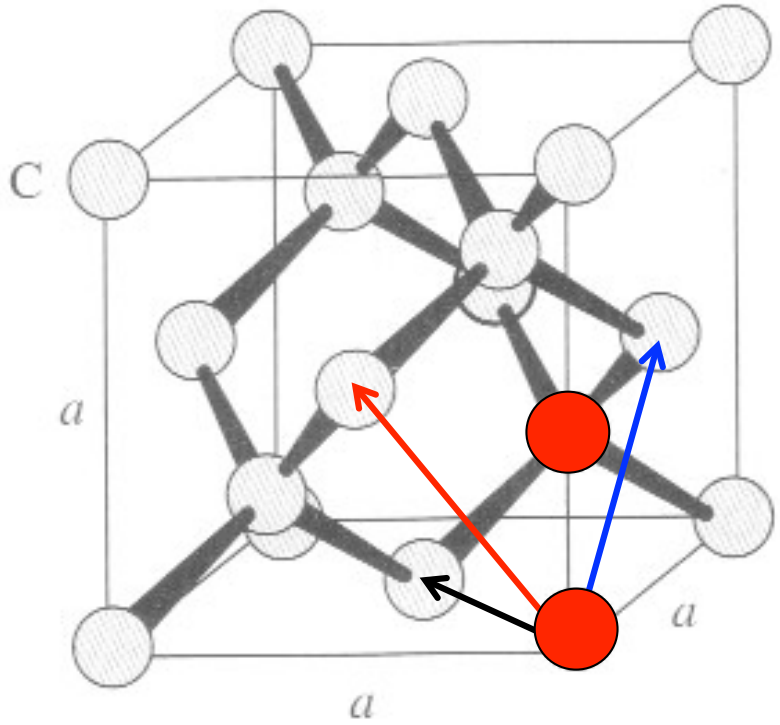

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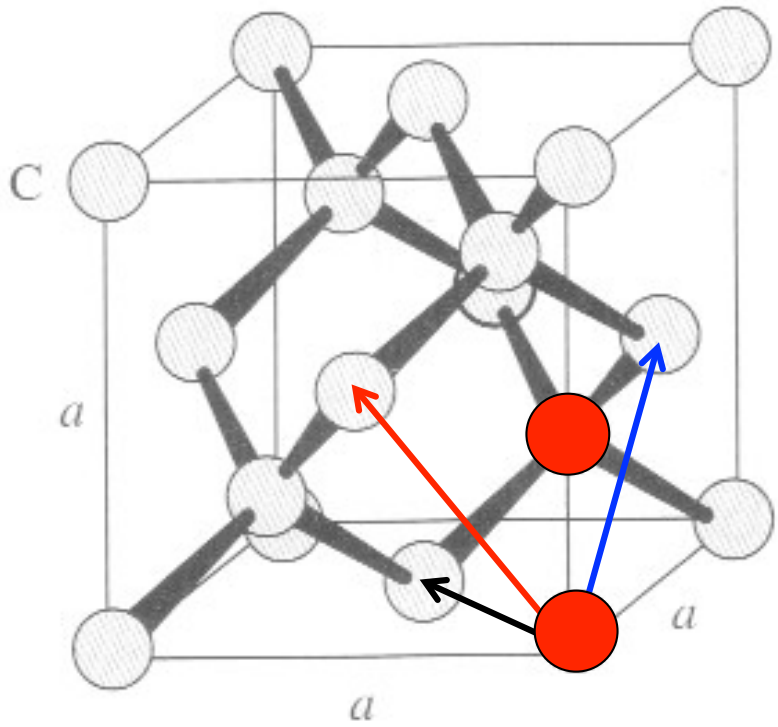

Name of the PP file

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

```
&control
   pseudo_dir='/where/my/pseudos/are'
/
```

Structure of QE input file

```
&control
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&system
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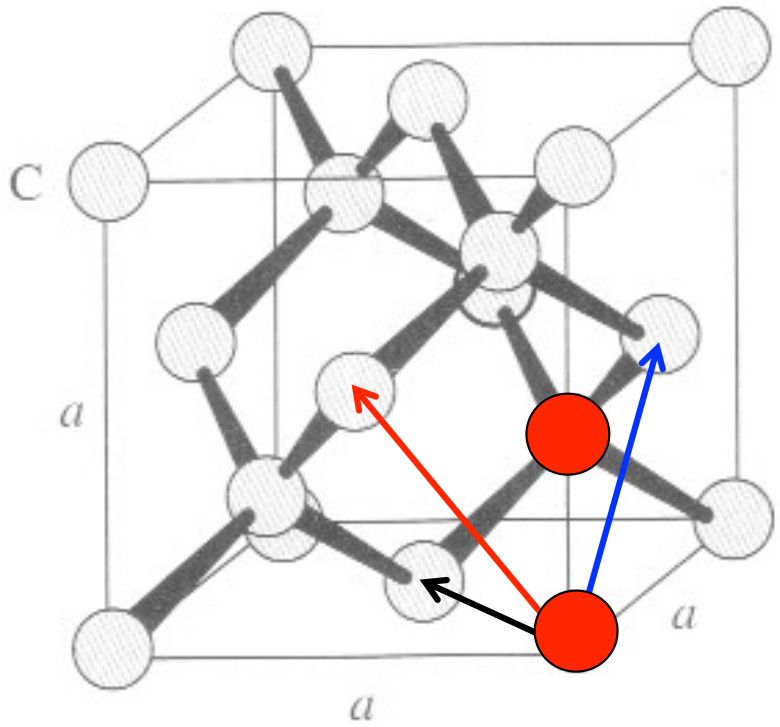
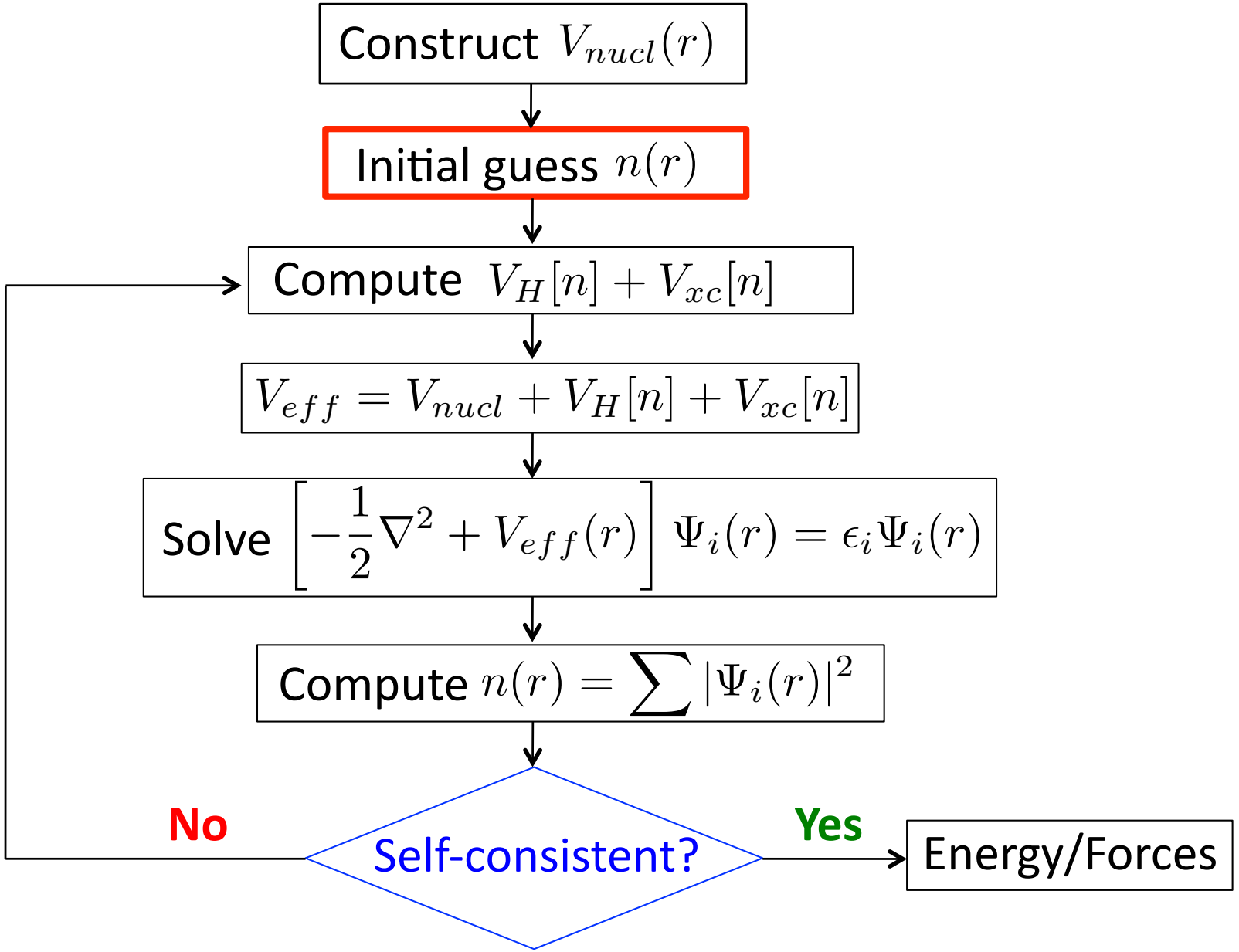


(alat, bohr, angstrom, crystal)

Iterative solution of KS equations



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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
```

startingwfc = ‘atomic’ (DEFAULT)
= ‘random’
= ‘file’

Plane wave expansion

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

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

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

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

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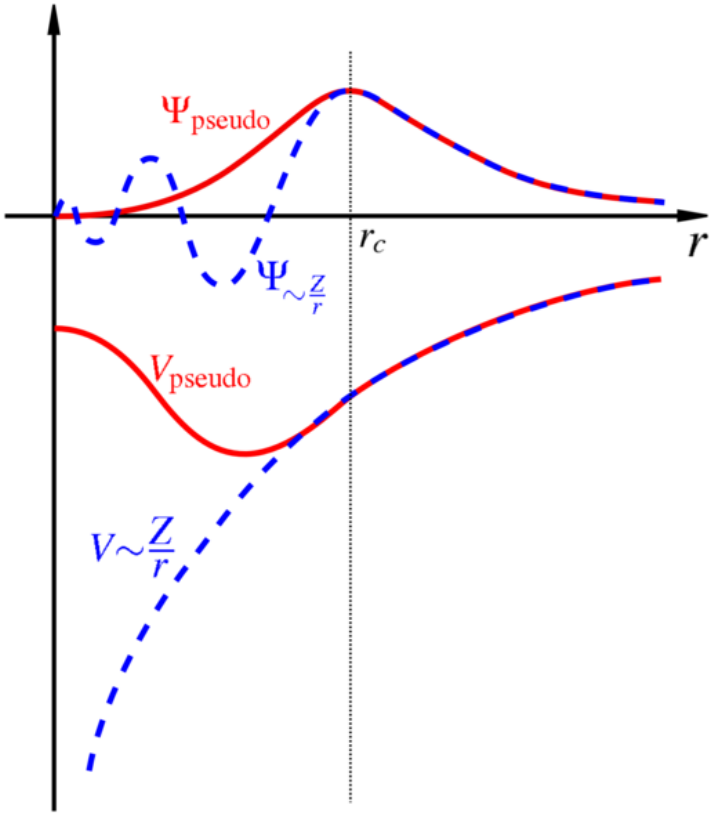

Problems:
1) Core electrons are localized
2) Valence electrons have nodes close to the nucleus

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

Pseudopotentials: The choice of E_{cut} depends on the PP

Structure of QE input file

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 Si 0.25 0.25 0.25
K_POINTS (automatic)
 6 6 6 1 1 1
```

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

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

For ultrasoft pseudopotentials we have also:
ecutrho = usually 8-12 * ecutwfc

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 Si 0.0 0.0 0.0
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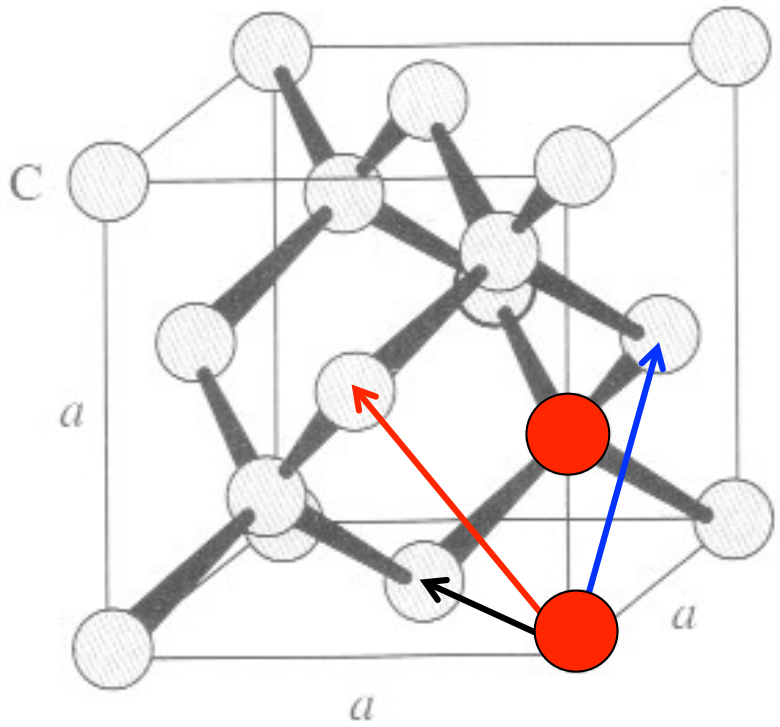

Name of the PP file: Si.pbe-rrkj.UPF

Pseudopotentials

```
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Generated using Andrea Dal Corso code (rrkj3)
Author: Andrea Dal Corso   Generation date: unknown
Info:   Si PBE 3s2 3p2 RRKJ3
   0       The Pseudo was generated with a Non-Relativistic Calculation
 2.50000000000E+00    Local Potential cutoff radius
nl pn  l   occ            Rcut          Rcut US          E pseu
3S  1  0  2.00     2.50000000000     2.60000000000     0.00000000000
3S  1  0  0.00     2.50000000000     2.60000000000     0.00000000000
3P  2  1  2.00     2.50000000000     2.70000000000     0.00000000000
3D  3  2  0.00     2.50000000000     2.50000000000     0.00000000000
</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     Z valence
  -7.47480832270     Total energy
 0.0000000  0.0000000 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>
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 1.77053726905E-04  1.79729551320E-04  1.82445815642E-04  1.85203131043E-04
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 1.99627519645E-04  2.02644503249E-04  2.05707082721E-04  2.08815947154E-04
 2.11971796056E-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
...
```

SEARCH

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Forum

PSEUDOPOTENTIALS

- Admin PP Database
- More about pseudopotentials
- Naming convention for the pseudopotential
- Unified Pseudopotential Format

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.

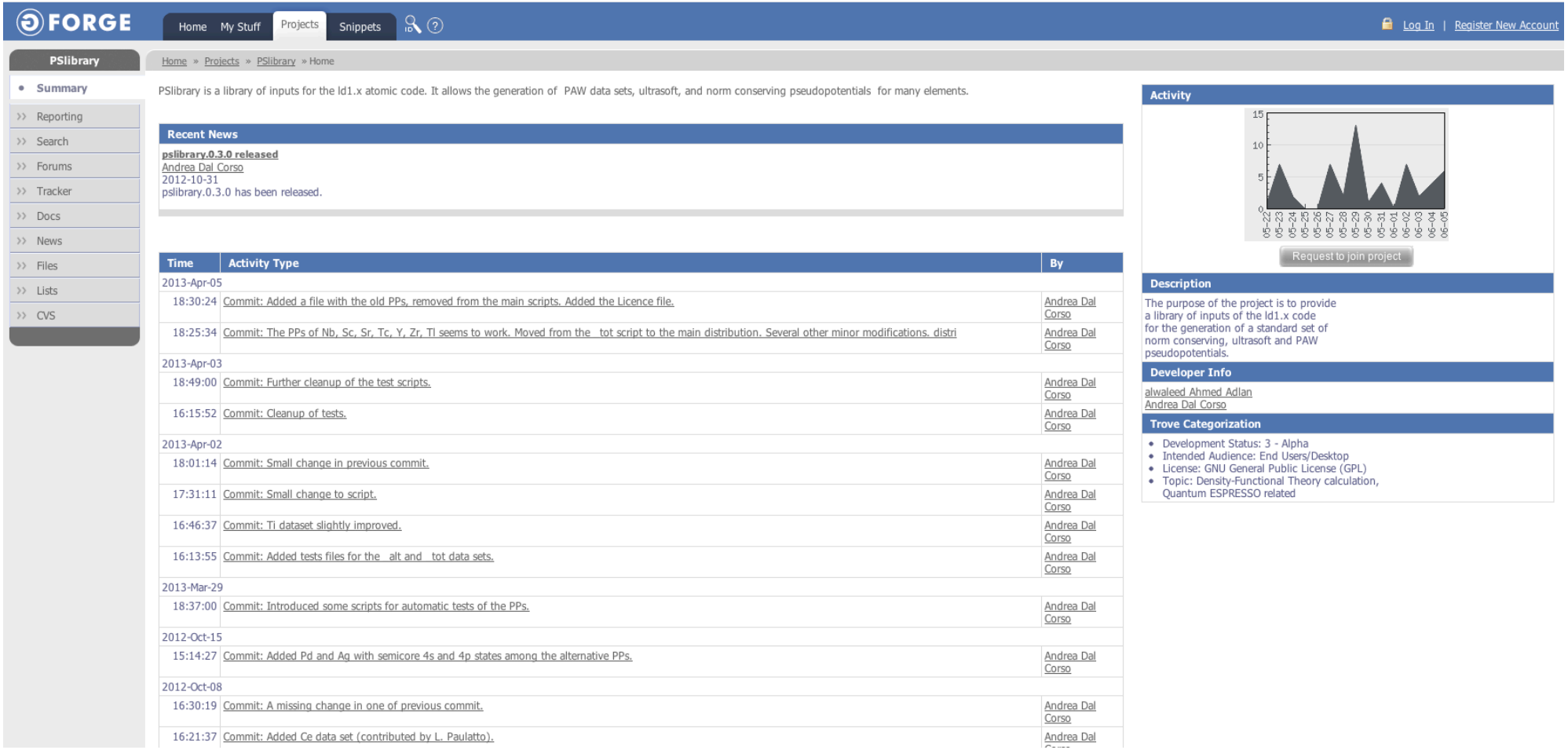
ANY FUNCTIONAL | ANY TYPE | Apply Filter

ANY PP LIBRARY | OTHER OPTIONS

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca		21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr		39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57-70 *	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89-102 **	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt									

* Lanthanoids	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb
** Actinoids	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No

http://www.qe-forge.org/gf/project/pslibrary/



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 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:

$$\overline{A} = \frac{1}{\Omega_{BZ}} \int_{BZ} A(\mathbf{k}) d\mathbf{k}$$

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

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

In practice the integral is discretized:

$$\frac{1}{\Omega_{BZ}} \int_{BZ} d\mathbf{k} \rightarrow \sum_{\mathbf{k}} \omega_{\mathbf{k}}$$

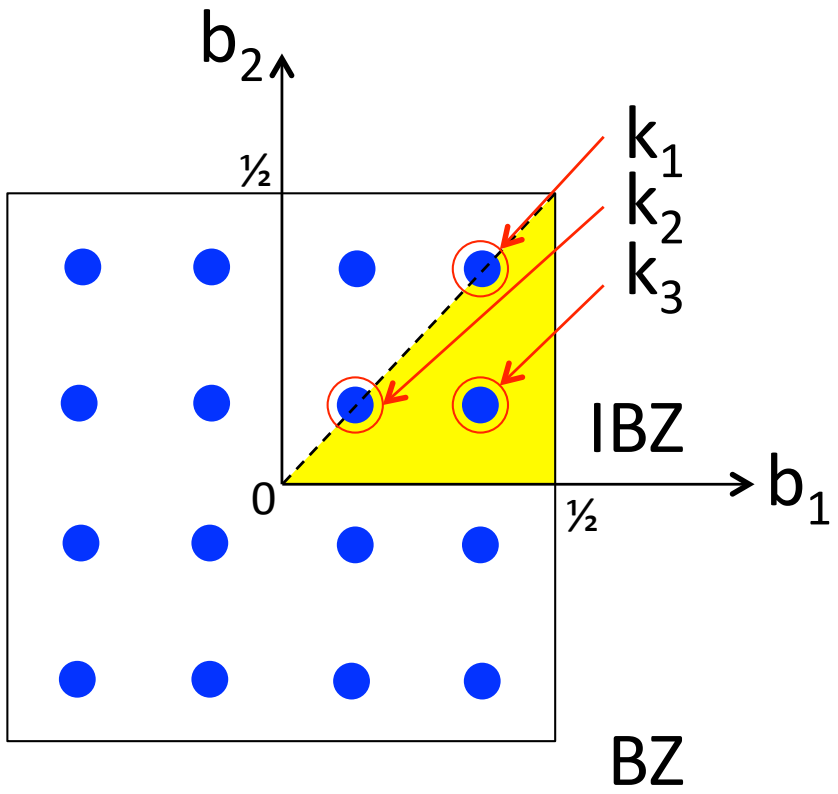
How do we choose the ***k*** points to include in the sum?

Sampling of the Brillouin zone

- example: square 2D lattice
- 4x4 k-points grid (16 points)

- 3 inequivalent points (IBZ)

  - 4 x k_1 --> $\omega_1 = ¼$
  - 4 x k_2 --> $\omega_2 = ¼$
  - 8 x k_3 --> $\omega_3 = ½$

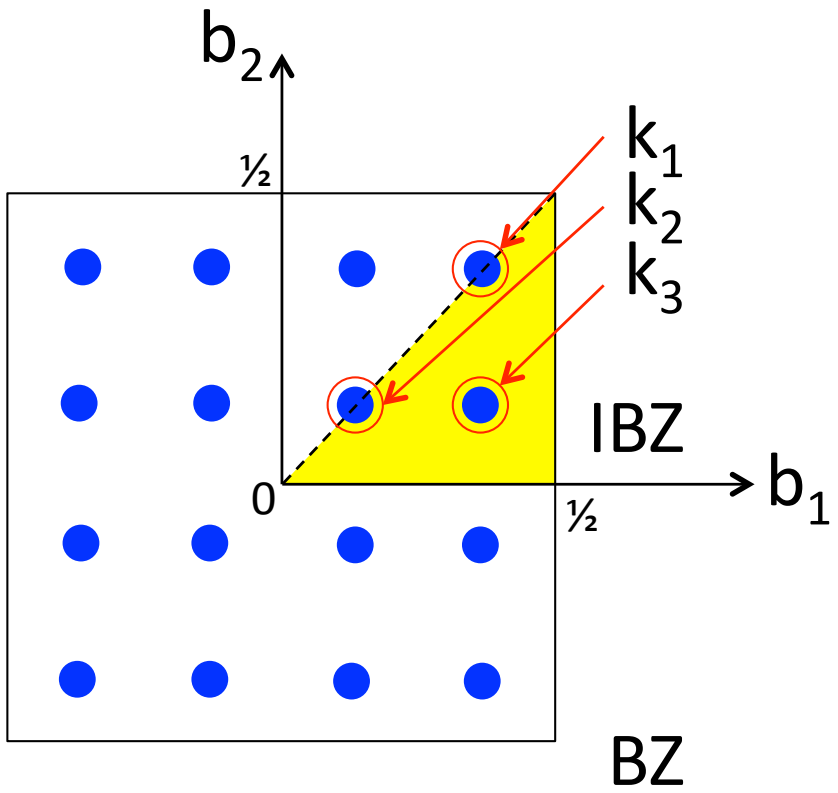


$$\frac{1}{\Omega_{BZ}} \int_{BZ} A(\mathbf{k}) d\mathbf{k} \simeq \frac{1}{4} A(\mathbf{k_1}) + \frac{1}{4} A(\mathbf{k_2}) + \frac{1}{2} A(\mathbf{k_3})$$

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
```

(automatic, tpiba, crystal, gamma)



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 Si 0.25 0.25 0.25
K_POINTS (automatic)
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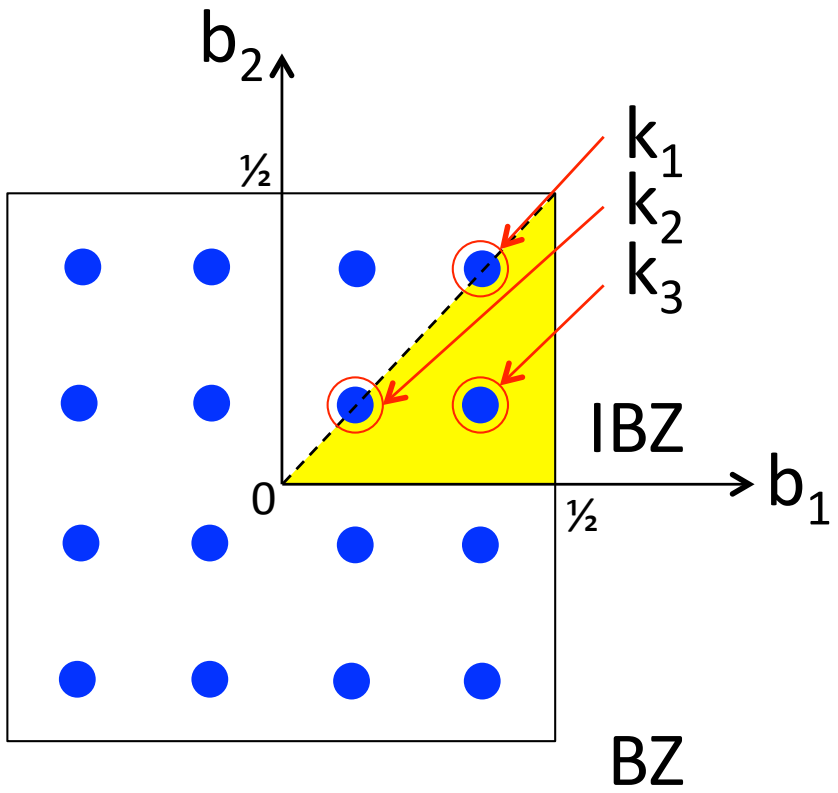
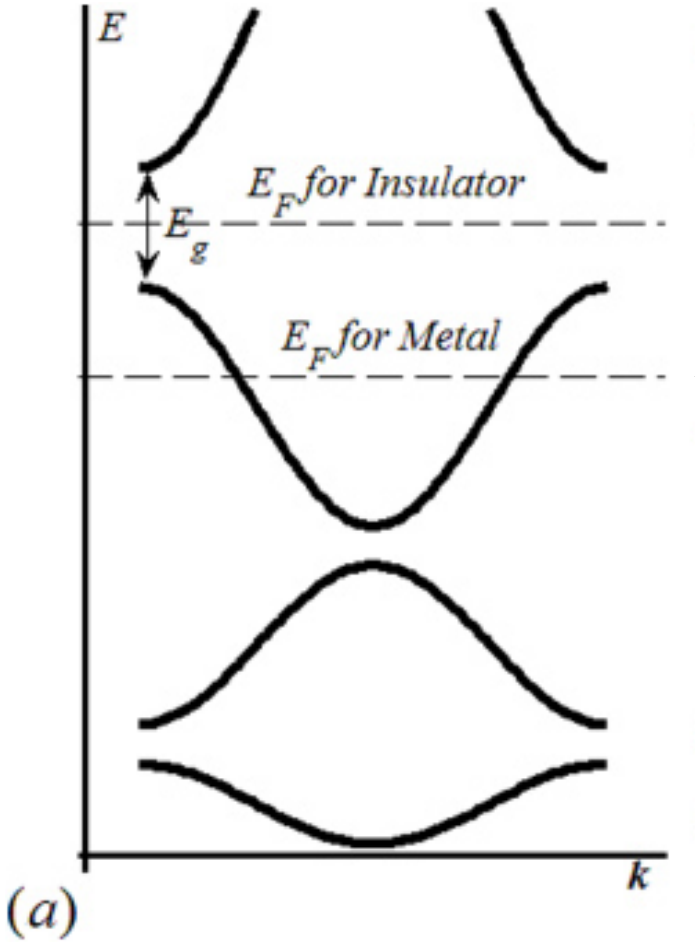


Nk1, NK2, NK3, shift1, shift2, shift3
shift: 0 or 1

Sampling of the Brillouin zone



← Discontinuity of occupations

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

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

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

σ : dimensions of energy,
controls the broadening of the Fermi surface
"smearing" of the Fermi surface

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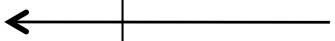
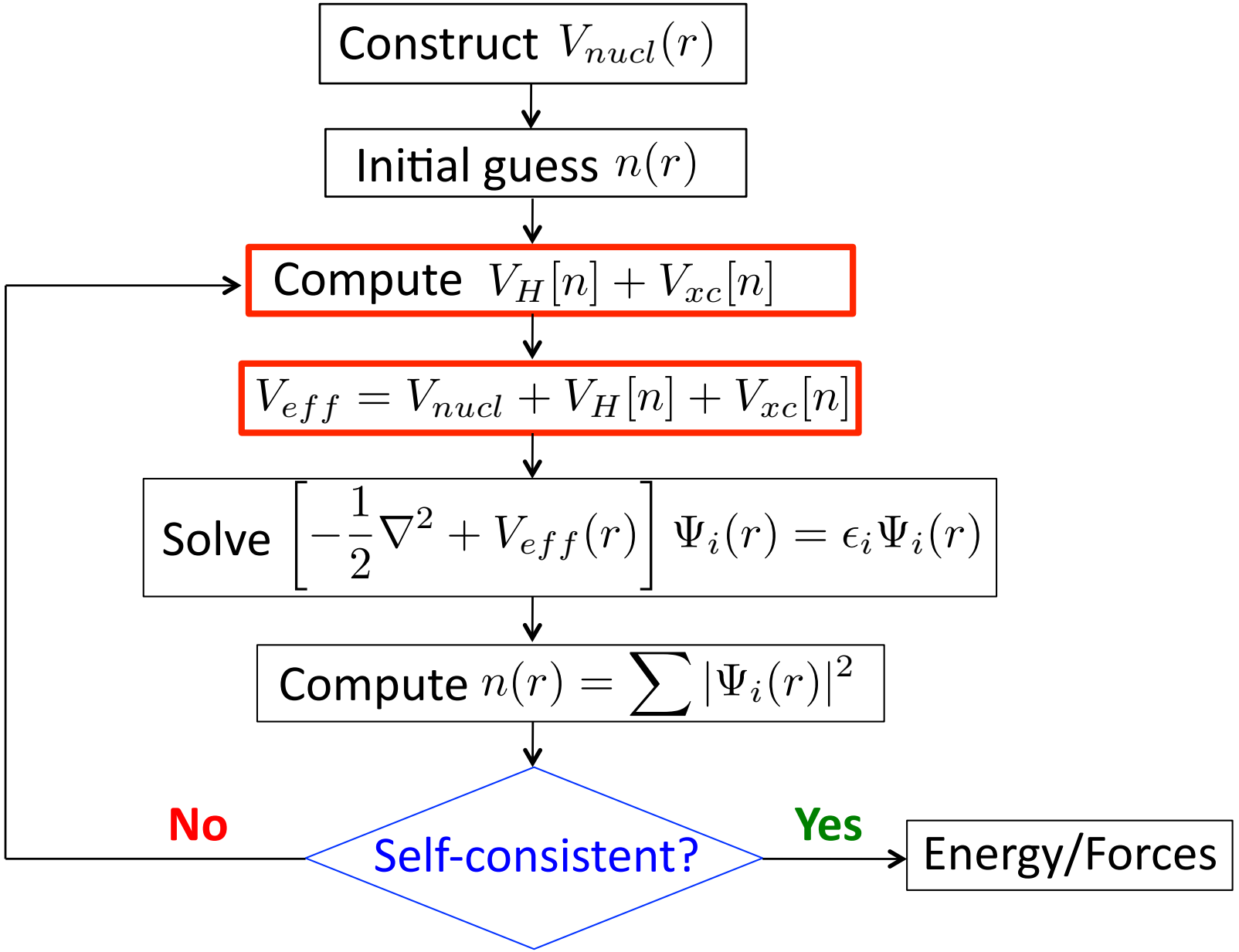
ATOMIC_POSITIONS (alat)
 Si 0.0 0.0 0.0
 Si 0.25 0.25 0.25
K_POINTS (automatic)
 6 6 6 1 1 1
```



occupations = ‘smearing’
smearing = ‘gaussian’ (or mp, mv, fd)
degauss = 0.01 (units: Ry)

Iterative solution of KS equations



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 Si 28.086  Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
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 Si 0.25 0.25 0.25
K_POINTS (automatic)
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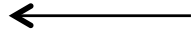
```



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

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&control
   calculation = 'scf',
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/
&system
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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
```

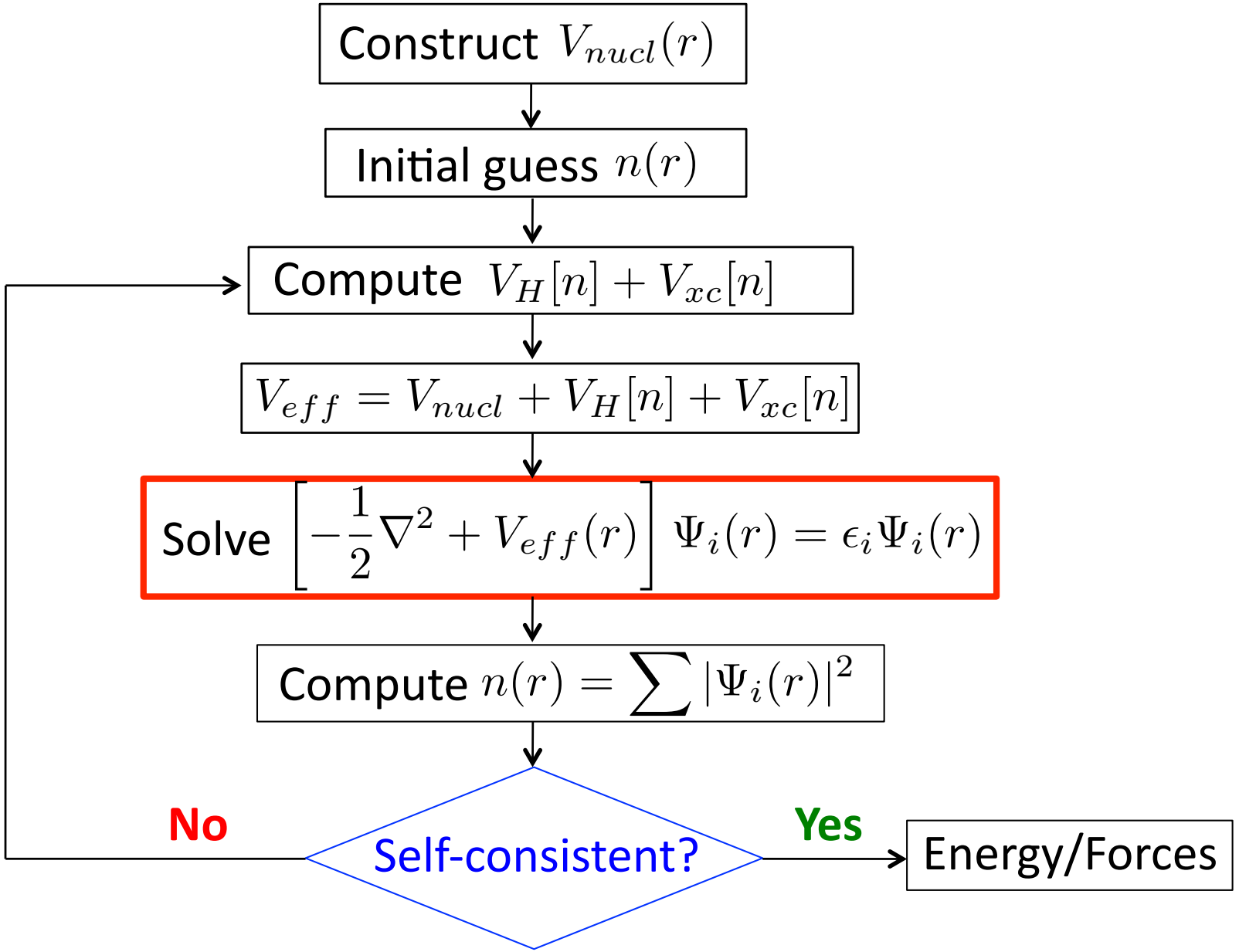
input_dft = 'rpbe'
= 'pz'
= 'b3lyp'
= … (see espresso-5.0.2/Modules/funct.f90)

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



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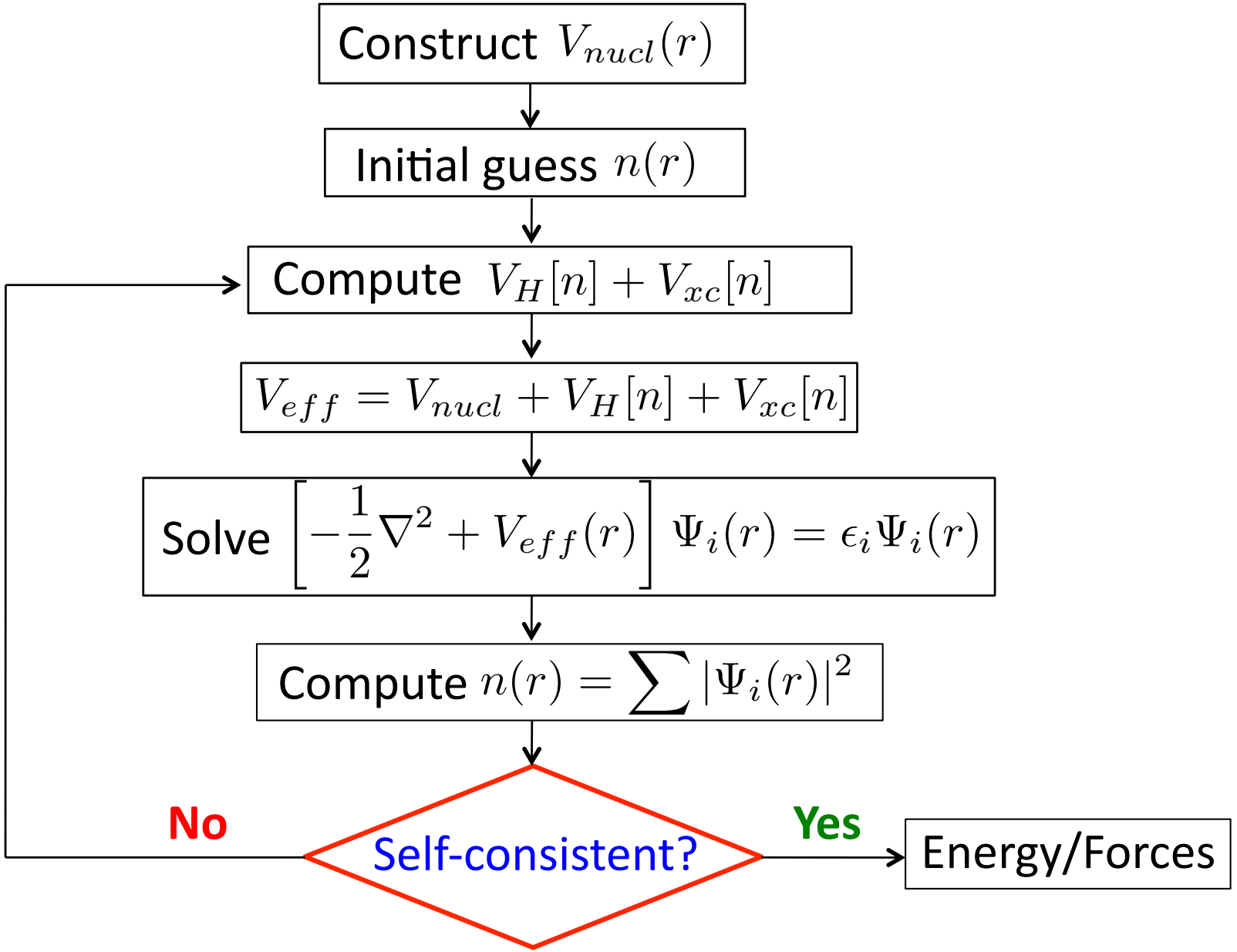
/
&system
   ibrav =  2,
   celldm(1) = 10.26,
   nat =  2,
   ntyp = 1,
   ecutwfc = 20
/
&electrons
   mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086  Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
 Si 0.0 0.0 0.0
 Si 0.25 0.25 0.25
K_POINTS (automatic)
 6 6 6 1 1 1
```

diagonalization = ‘david’ (DEFAULT)
= ‘cg’

Iterative solution of KS equations



Structure of QE input file

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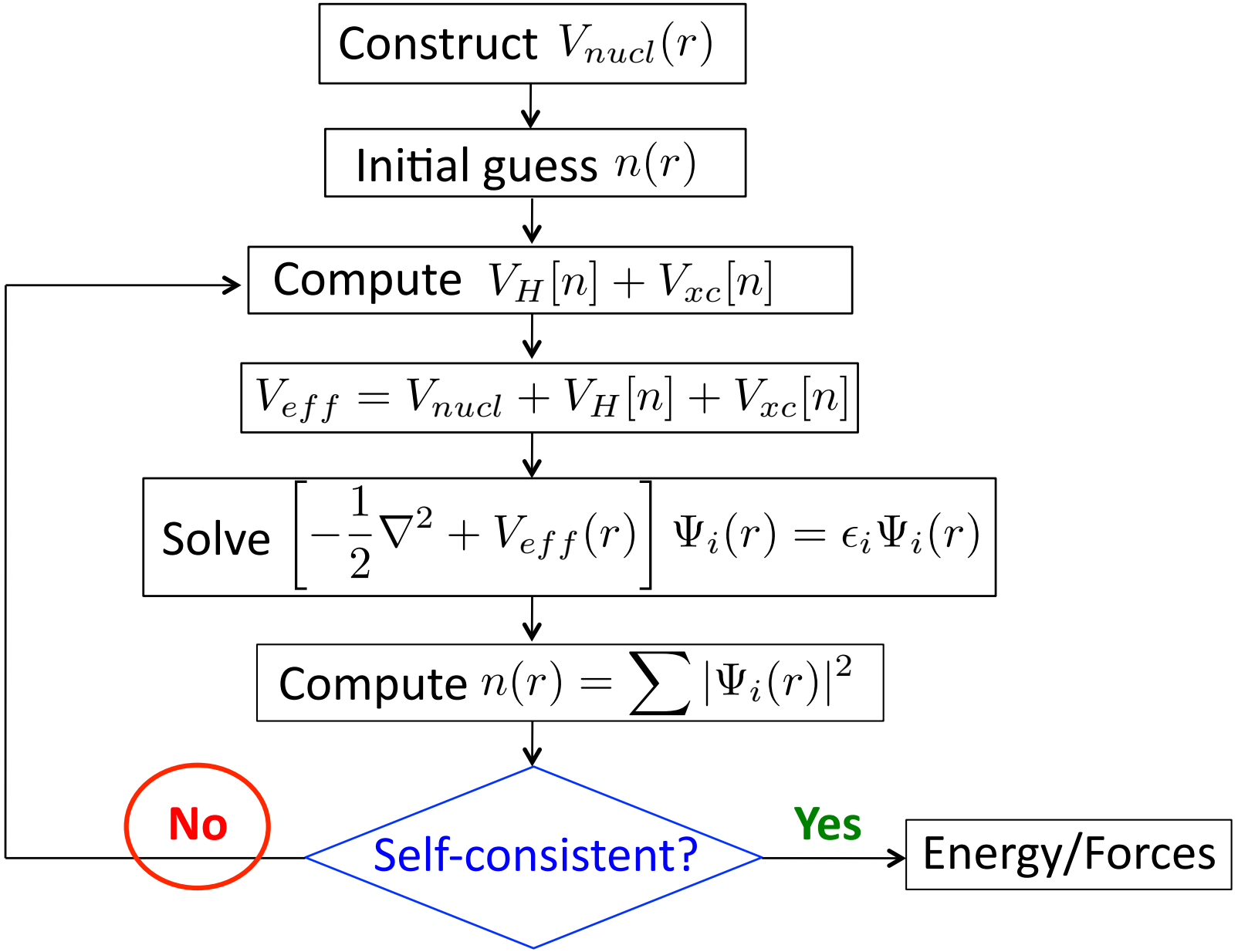
   ntyp = 1,
   ecutwfc = 20
/
&electrons
   mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086  Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
 Si 0.0 0.0 0.0
 Si 0.25 0.25 0.25
K_POINTS (automatic)
 6 6 6 1 1 1
```

conv_thr = 1.d-6 (DEFAULT)
= 1.d-8

Iterative solution of KS equations

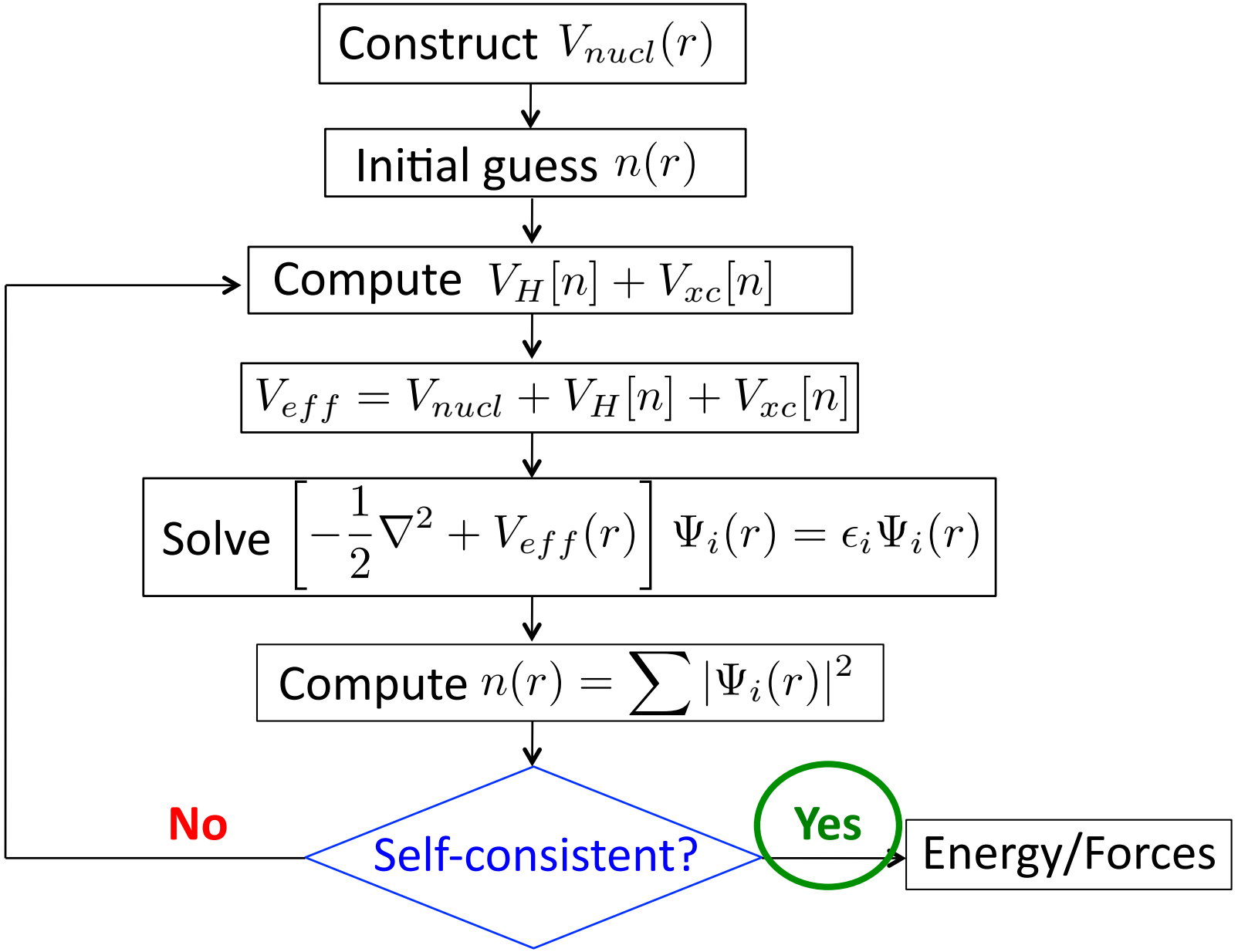


Mixing

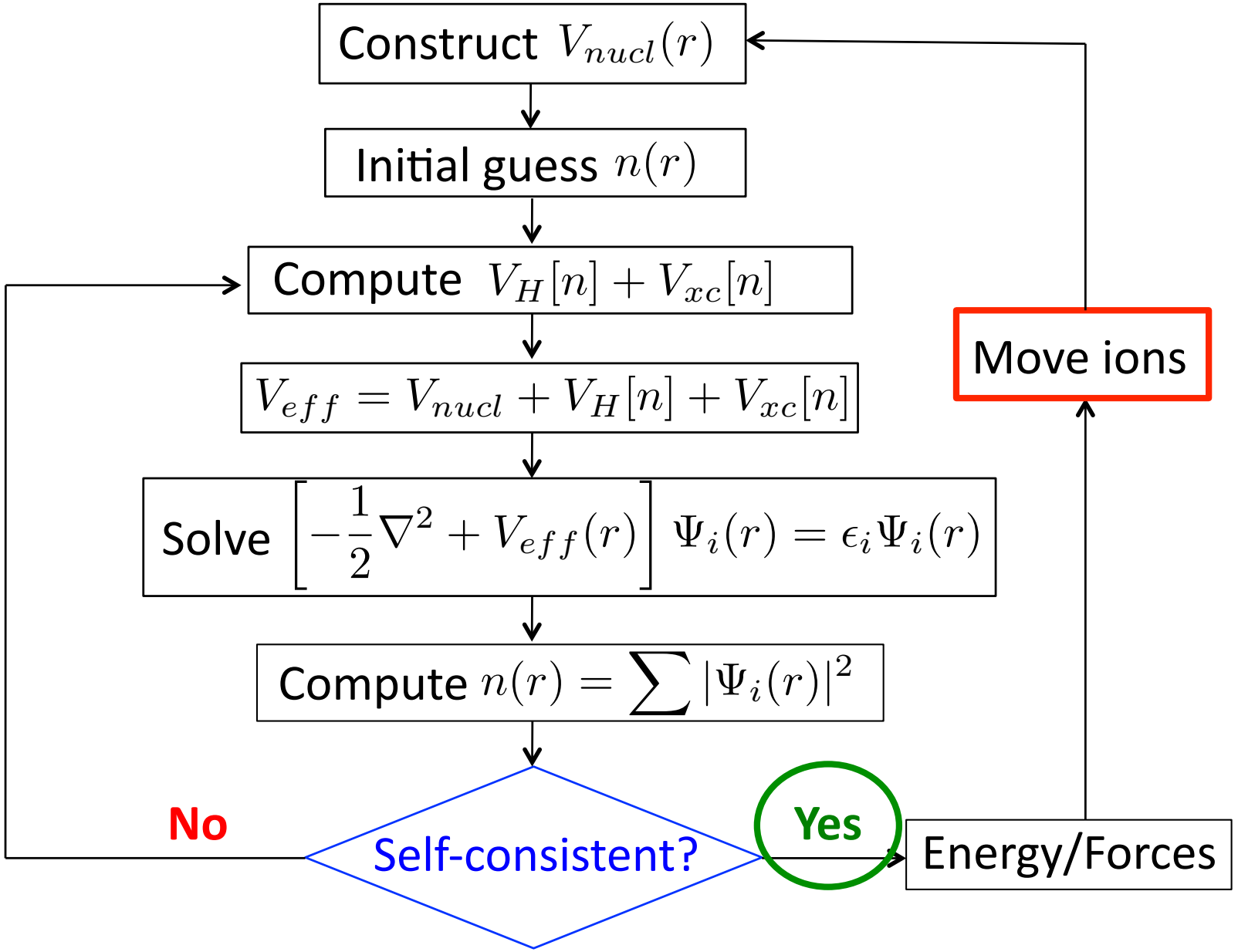
```
&control
   calculation = 'scf',
   prefix = 'Si_exc1',
/
&system
   ibrav =  2,
   celldm(1) = 10.26,
   nat =  2,
   ntyp = 1,
   ecutwfc = 20
/
&electrons
   mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086  Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
 Si 0.0 0.0 0.0
 Si 0.25 0.25 0.25
K_POINTS (automatic)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

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

Iterative solution of KS equations



Iterative solution of KS equations



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,
/
…
```

← (or ‘damp’, ‘verlet’, ‘langevin’)

← (DEFAULT: ‘none’)

← (DEFAULT: ‘none’)

← (DEFAULT: 10)

Exercises

Read the instructions !!!

Exercise 1: bulk Si

- convergence of Etot w.r.t. plane waves cutoff (ecutwfc)
- convergence of Etot w.r.t. BZ sampling (K_POINTS)
- lattice constant

Exercise 2: bulk Al (metal!)

- convergence of Etot w.r.t. plane waves cutoff (ecutwfc)
- convergence of Etot w.r.t. BZ sampling (K_POINTS)
- lattice constant