DFT Simulation with Quantum Espresso

Psi-K Quantum-ESPRESSO School on Ab-Initio Thermal Transport

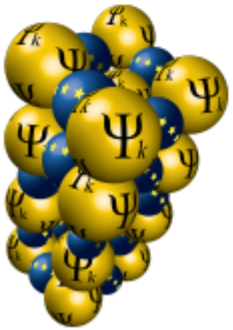
Lorenzo Paulatto

IMPMC – Institut de minéralogie, de physique des matériaux et de cosmochimie
UMR 7590 - UPMC/CNRS/IRD/MNHN

UPMC – Université Pierre-et-Marie-Curie - Sorbonne Universités
CNRS – Centre national de la recherche scientifique

lorenzo.paulatto@impmc.upmc.fr

June 27, 2016



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25.04.16

QUANTUM ESPRESSO V5.4.0

Version 5.4.0 of Quantum ESPRESSO is available for download. You can find all archives uploaded on QE-FORGE here.

31.01.16

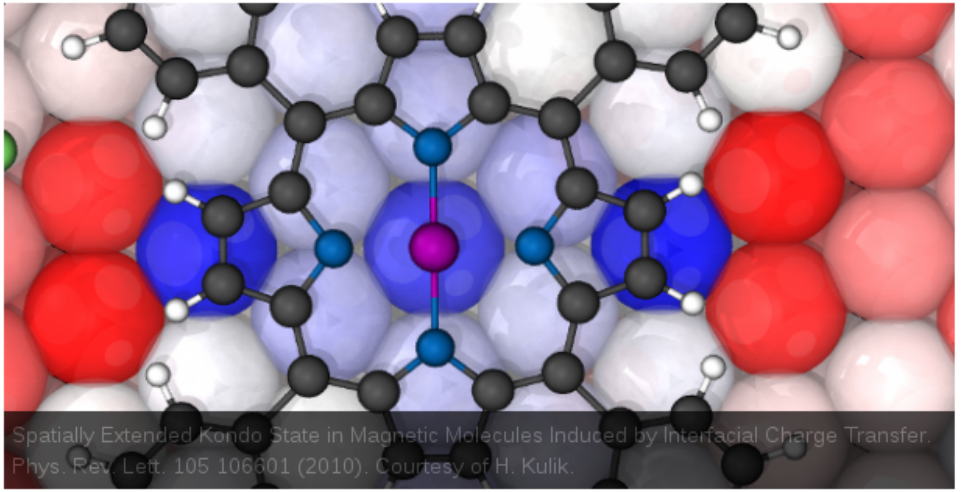
THE WALTER KOHN PRIZE

A prize for outstanding contributions in the field of quantum-mechanical materials and molecular modeling. More information here.

11.01.16

QUANTUM ESPRESSO V5.3.0

Version 5.3.0 of Quantum ESPRESSO is available for download.



Spatially Extended Kondo State in Magnetic Molecules Induced by Interfacial Charge Transfer. Phys. Rev. Lett. 105 106601 (2010). Courtesy of H. Kulik.

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.

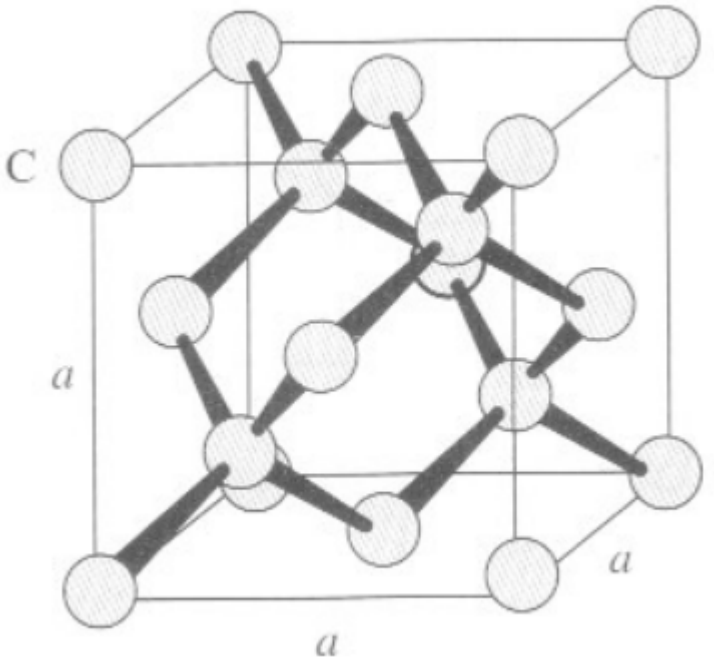
READ MORE >

What I cannot compute, I do not understand (adapted from Richard P. Feynman)

Adapted by R. Sabatini on WordPress

Quantum-ESPRESSO input file

```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
/
&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.   0.   0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```



Quantum-ESPRESSO input file

```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
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    ecutwfc = 16.0
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&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.   0.   0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```
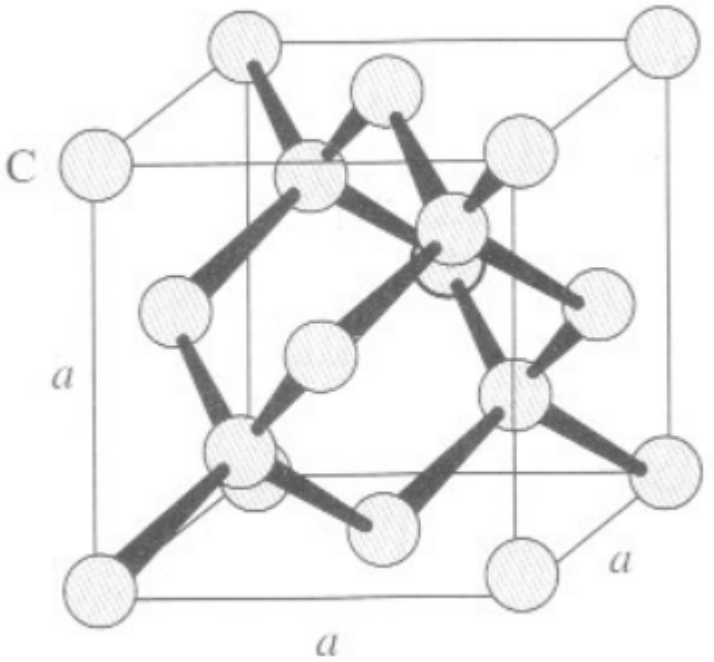



The Kohn-Sham Problem

The Kohn-Sham Equation

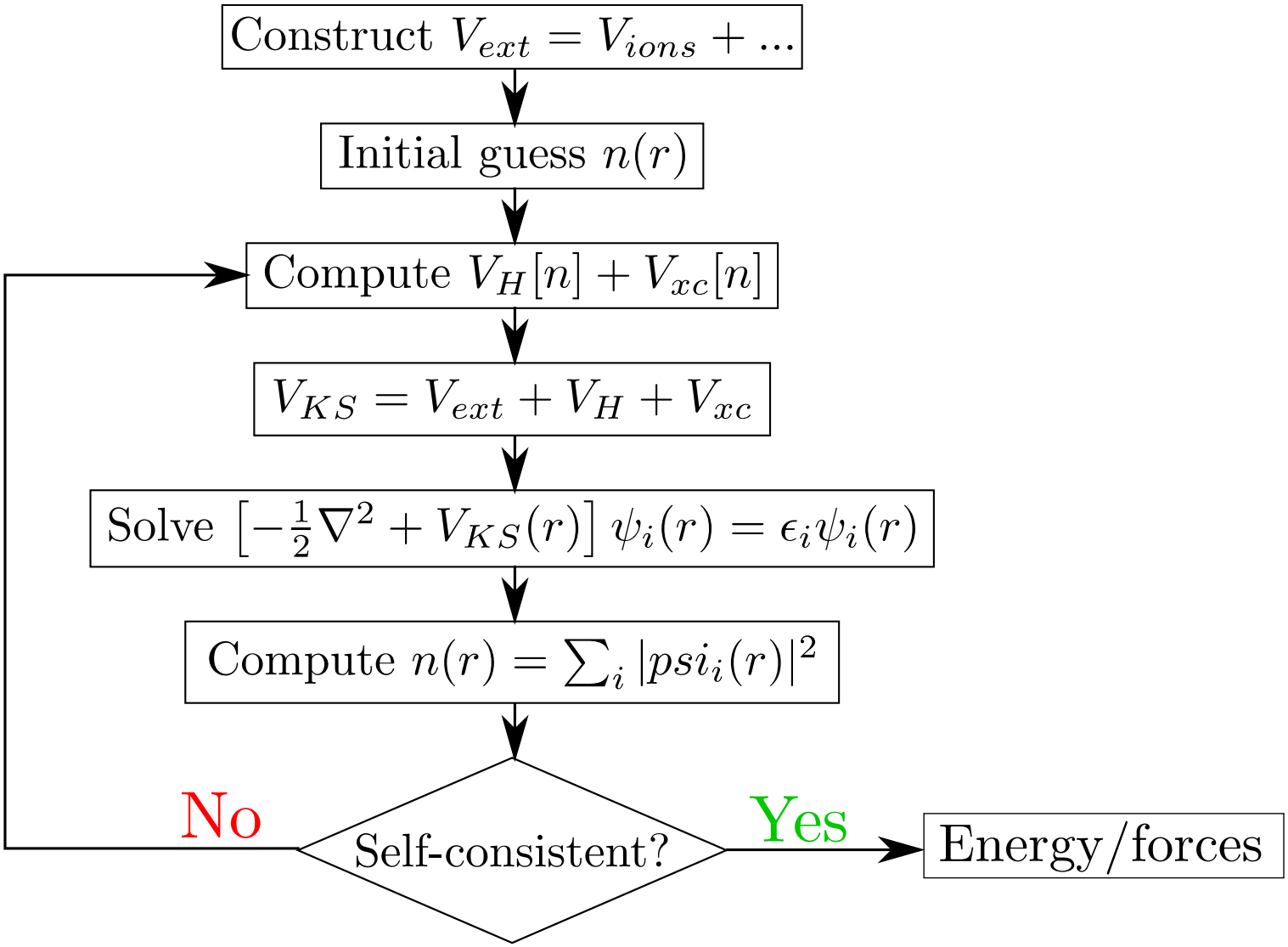
$$\left[-\frac{1}{2}\nabla^2 + V_{ext} + V_H[n] + V_{xc}[n]\right]\psi_i(r) = \epsilon_i\psi_i(r)$$

Self-Consistent Field procedure

$$\psi_i(r) \longrightarrow n(r) \longrightarrow H[n]$$

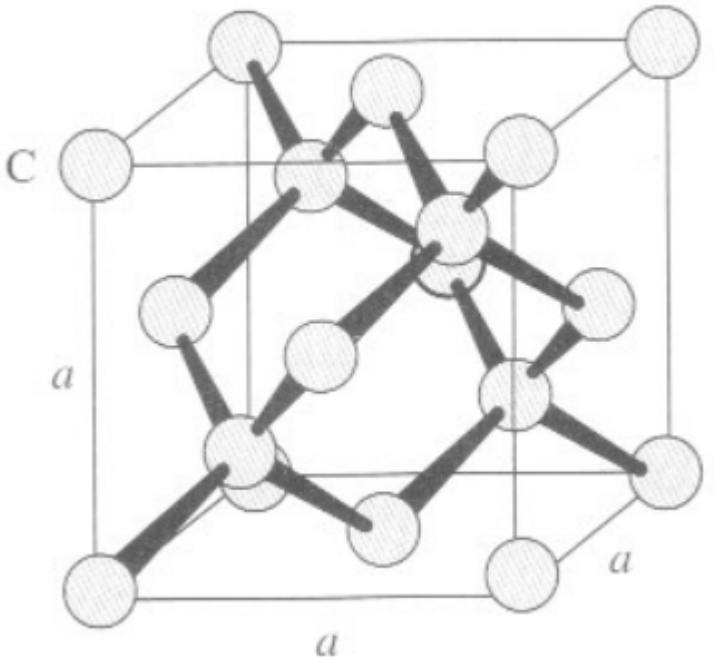
Computed by the pw.x code of QE

Iterative Solution of the Kohn-Sham Equations



Quantum-ESPRESSO input file

```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
/
&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.   0.   0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```

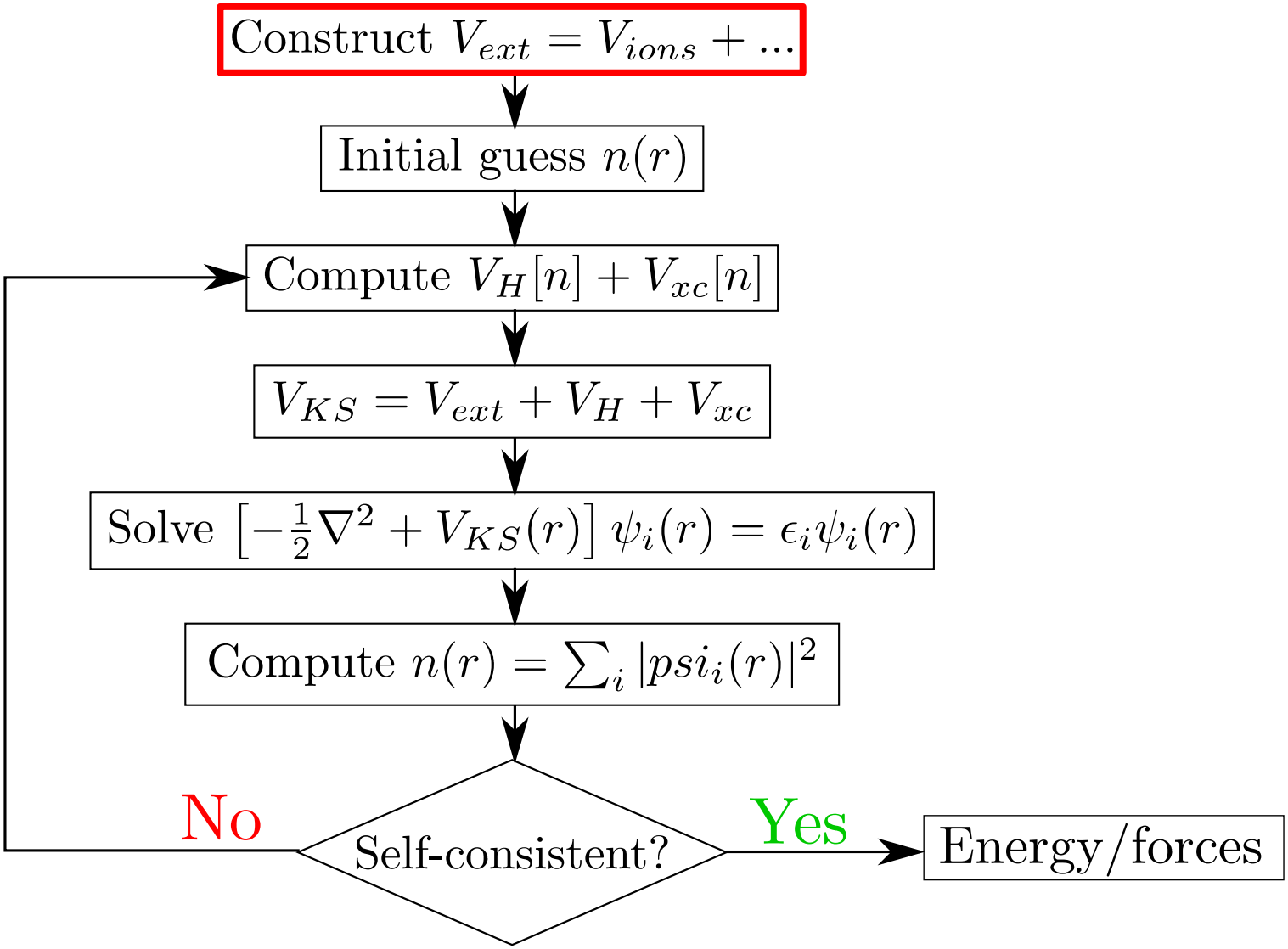


Quantum-ESPRESSO input file

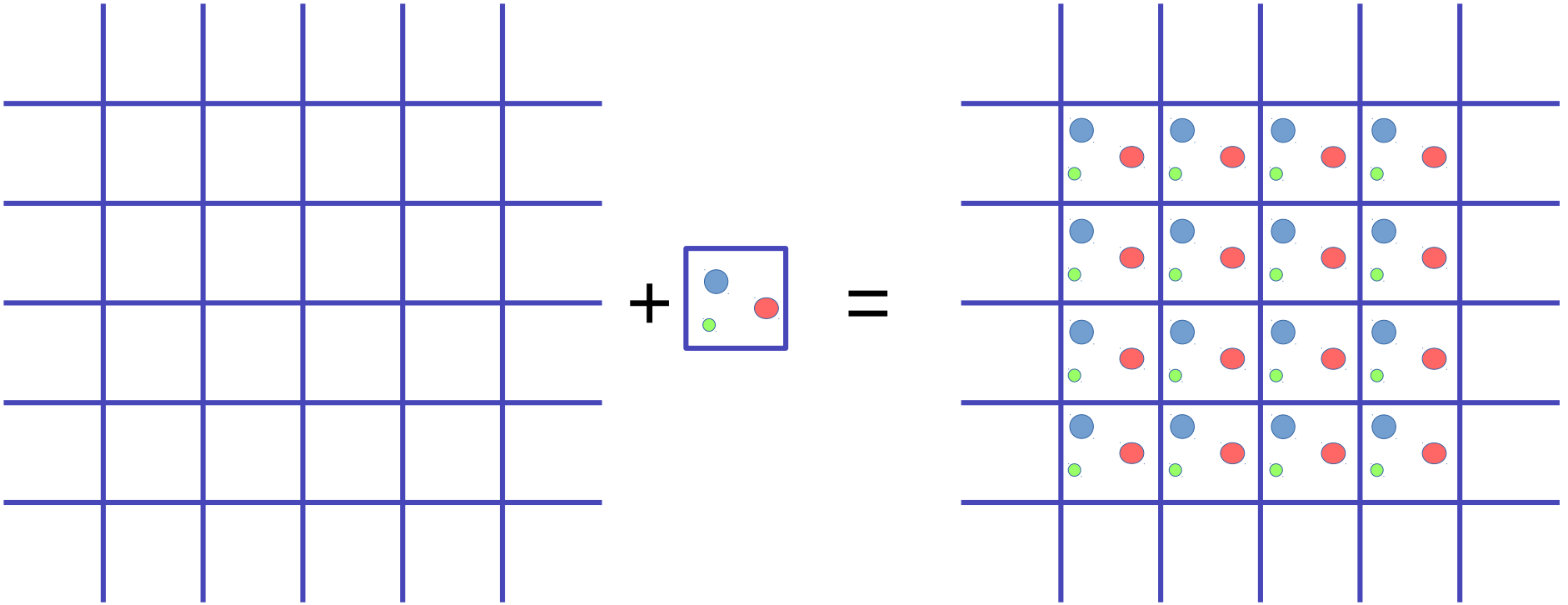
```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
/
&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.   0.   0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```

= "scf", "nscf", "relax", "md"

Iterative Solution of the Kohn-Sham Equations



Crystal Lattice and Basis



Periodic System = Lattice + Basis

Quantum-ESPRESSO input file

```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
/
&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.    0.    0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```

```
ibrav = 1: simple cubic
        2: fcc
        4: hexagonal
        0: manual
...
```

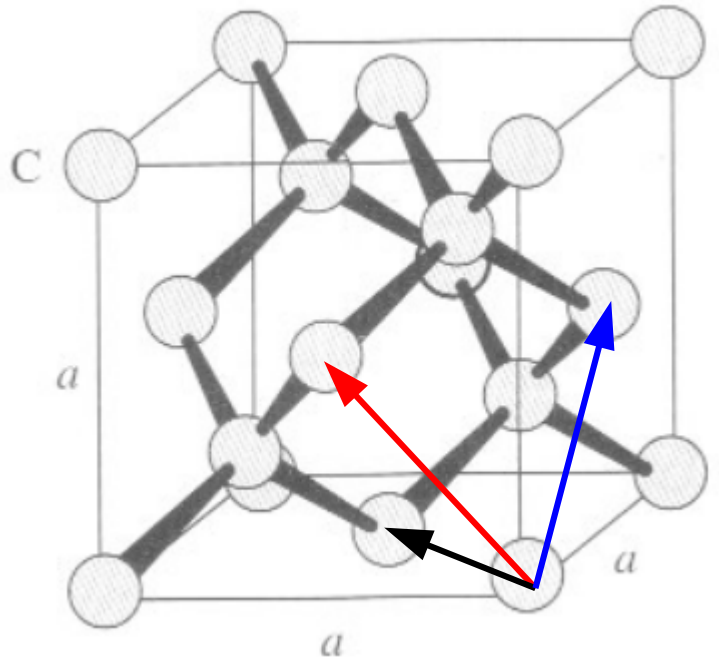
simple cubic:
a1 = a(1,0,0), a2=(0,1,0), a3=(0,0,1)

fcc:
a1=(a/2)(-1,0,1), a2=(a/2)(0,1,1), a3=(a/2)(-1,1,0)

hexagonal:
a1=a(1,0,0), a2=a(-1/2,sqrt(3)/2,0) a3=a(0,0,c/a)

Quantum-ESPRESSO input file

```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
/
&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.   0.   0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```



fcc:
a1=(a/2)(-1,0,1), a2=(a/2)(0,1,1), a3=(a/2)(-1,1,0)

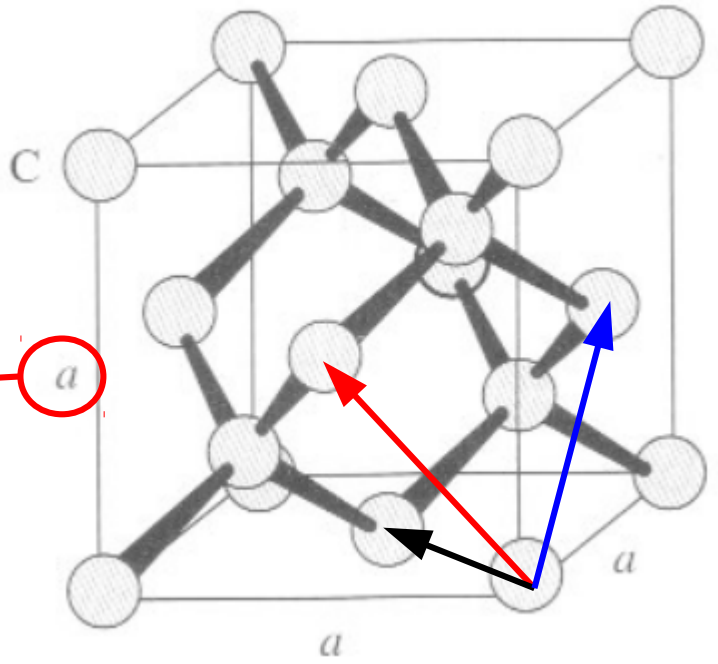
Quantum-ESPRESSO input file

```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
/
&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.   0.   0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```

alat, units: bohr (1 bohr = 0.521977 Å)

Quantum-ESPRESSO input file

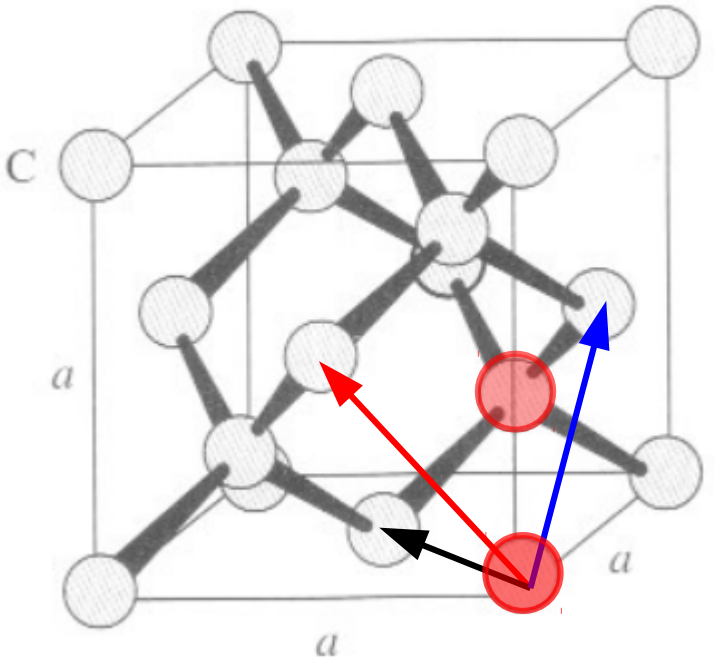
```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
/
&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.   0.   0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```



fcc:
a1=(a/2)(-1,0,1), a2=(a/2)(0,1,1), a3=(a/2)(-1,1,0)

Quantum-ESPRESSO input file

```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
/
&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.    0.    0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```

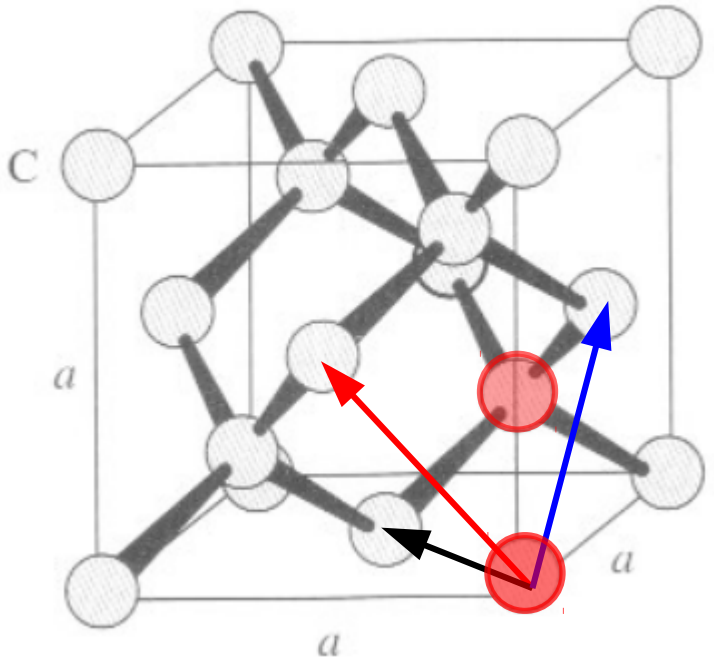


alat, crystal, bohr, angstrom

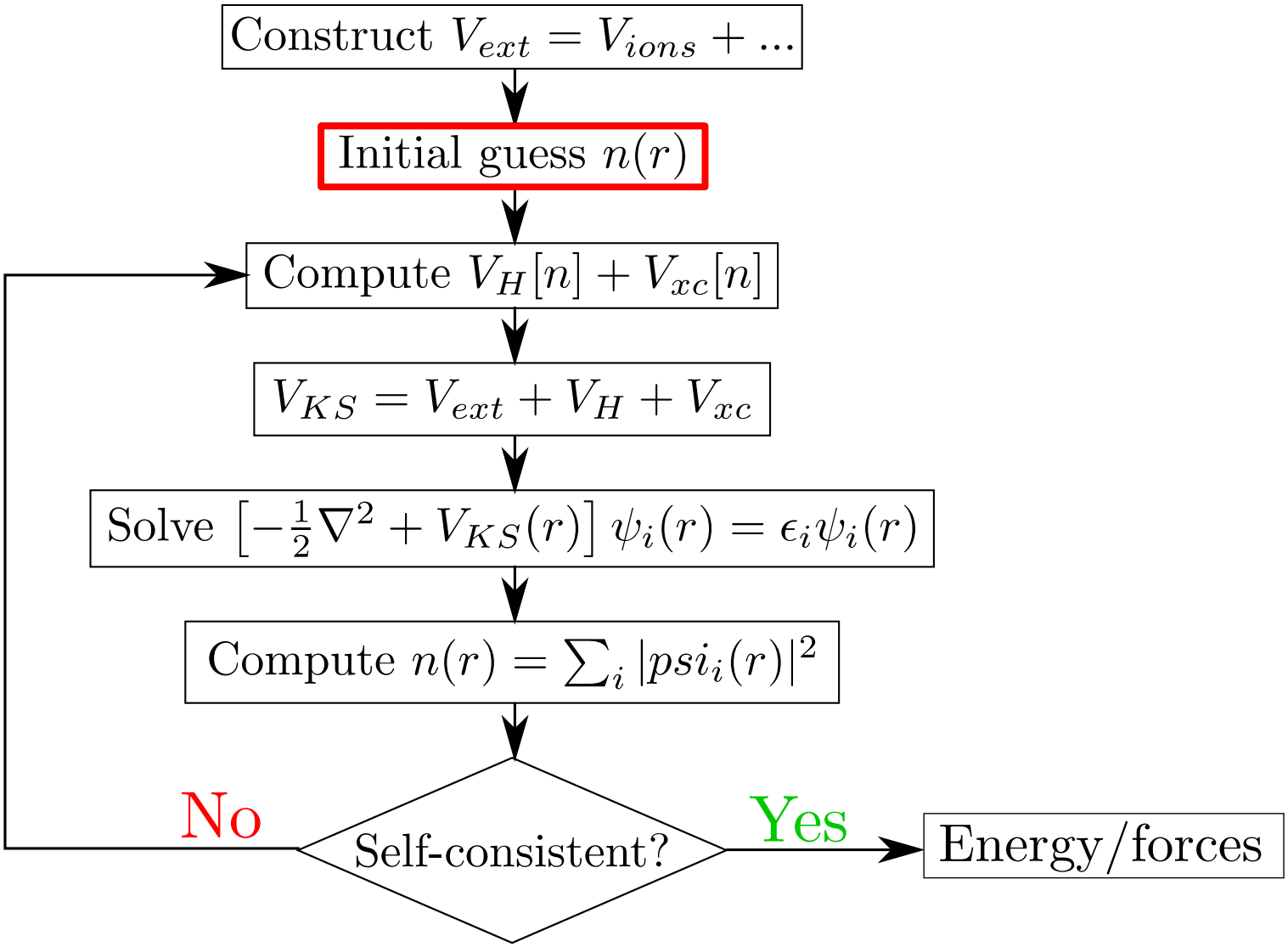
Simple mathematical expressions are allowed, i.e.
Si 1/4 1/4 1/4 (without spaces)

Quantum-ESPRESSO input file

```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
/
&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.   0.   0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```



Iterative Solution of the Kohn-Sham Equations



Quantum-ESPRESSO input file

```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
/
&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.   0.   0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```

= "atomic" (DEFAULT, if available)
= "random"
= "file"
= "atomic+random"

Quantum-ESPRESSO input file

```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
/
&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.    0.    0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```

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

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

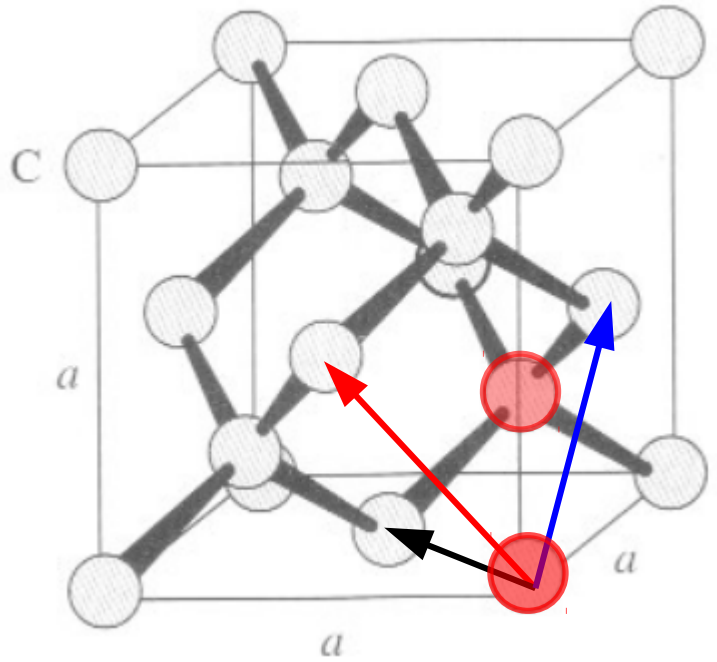
for ultrasoft pseudopotentials we have
ecutrho = usually 8-12 * ecutwfc (default 4*ecutwfc)

for PAW pseudopotentials
ecutrho = can be 4-8 * ecutwfc

TEST CONVERGENCE!!

Quantum-ESPRESSO input file

```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
/
&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.   0.   0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```



Name of the pseudopotential file:
Si.pz-rrkj.UPF

Pseudopotential UPF format

```
<UPF version="2.0.0">
  <PP_INFO>
    Generated using "atomic" code by A. Dal Corso (espresso distribution)
    Author: ADC
    Generation date: 24May2008
    Pseudopotential type: NC
    Element: Si
    Functional: LDA

    Suggested minimum cutoff for wavefunctions:  30. Ry
    Suggested minimum cutoff for charge density: 119. Ry
    The Pseudo was generated with a Scalar-Relativistic Calculation
    L component and cutoff radius for Local Potential:  2   2.4000

    Valence configuration:
    nl pn  l   occ       Rcut    Rcut US       E pseu
    3S  1  0  2.00      2.200      2.200    -0.799991
    3P  2  1  2.00      2.400      2.400    -0.306394
    Generation configuration:
    3S  1  0  2.00      2.200      2.200    -0.799990
    3P  2  1  2.00      2.400      2.400    -0.306394
    3D  3  2 -2.00      2.400      2.400     0.200000

    Pseudization used: rrkj
  </PP_INFO>
```

Pseudopotential libraries
http://www.quantum-espresso.org/pseudopotentials/

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PSEUDOPOTENTIALS

- Admin PP Database
- More about pseudopotentials
- Naming convention for the pseudopotential
- PSLibrary
- 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.

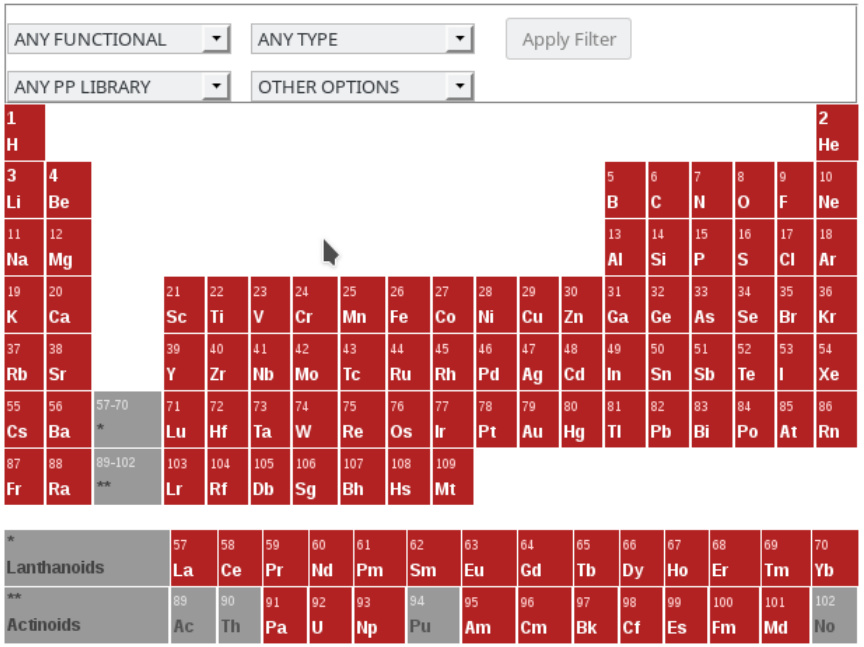
Standard Solid State Pseudopotentials (SSSP), a collection of the best verified pseudopotentials, maintained by THEOS and MARVEL, can be found, together with tests, on the Materials Cloud (materialscloud.org).

PAW datasets for rare earths can be found on the web page of VLab at University of Minnesota.

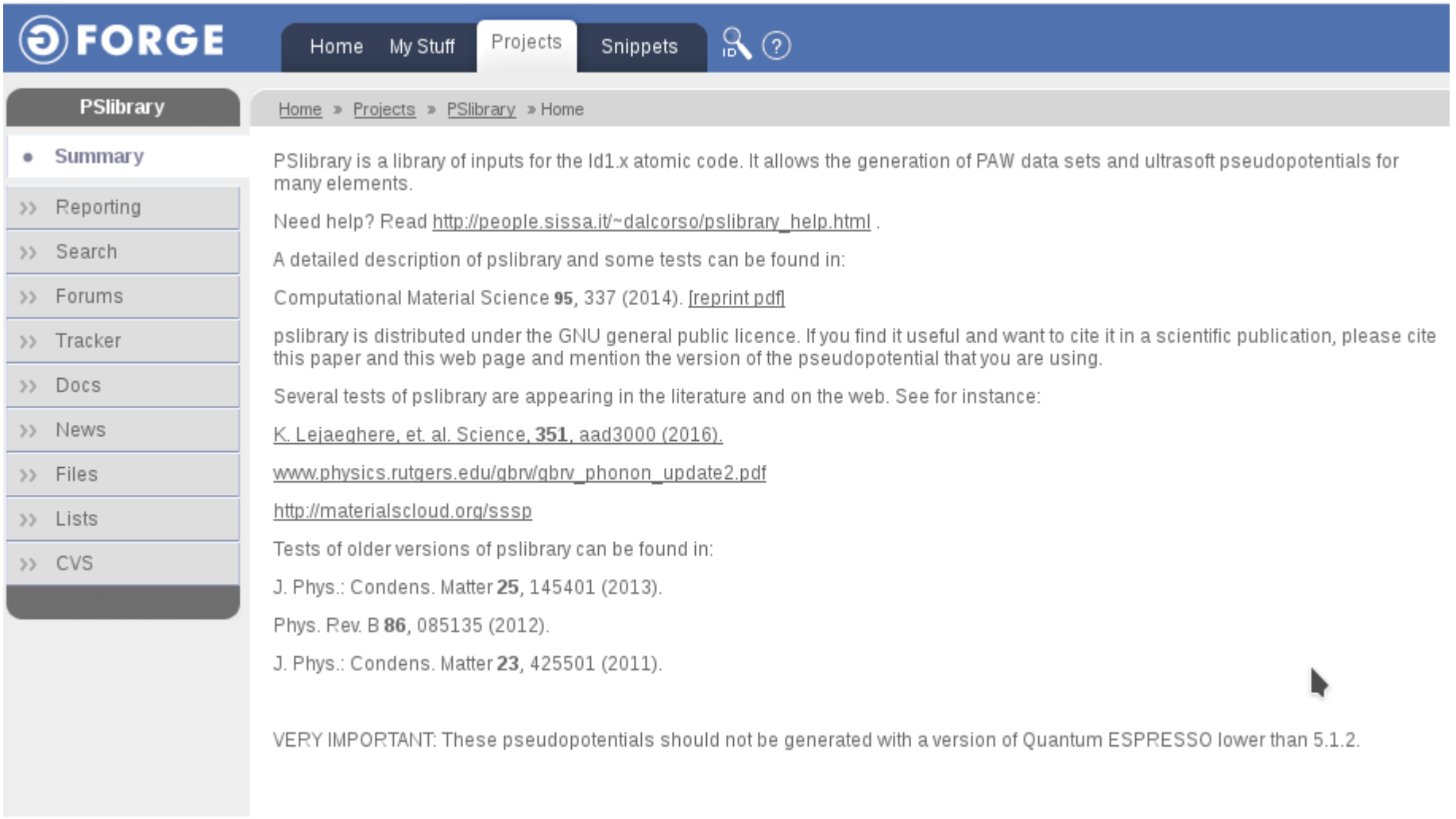
More information about pseudopotentials in general, the naming convention adopted for pseudopotential files, the Unified Pseudopotential Format , and on other pseudopotential databases, can be found via the links of the menu at the left.

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.

(last updated April 7, 2016)



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



Pseudopotential libraries
https://www.physics.rutgers.edu/gbrv/

GBRV
high-throughput
pseudopotentials

The State University of New Jersey
Rutgers
Department of Physics and Astronomy

by Kevin F. Garrity, Joseph W. Bennett, Karin M. Rabe, and David Vanderbilt

Updated September 23, 2015

Version 1.5 now available. See below, here(pdf) and here(pdf).

Welcome to the GBRV pseudopotential site. This site hosts the GBRV pseudopotential library, a highly accurate and computationally inexpensive open-source pseudopotential library which has been designed and optimized for use in high-throughput DFT calculations and released under the gnu public license. We provide potential files for direct use with the Quantum Espresso, Abinit, and JDFTx plane-wave pseudopotential codes, as well as input files for the Vanderbilt Ultrasoft pseudopotential generator. Please see our paper: K.F. Garrity, J.W. Bennett, K.M. Rabe and D. Vanderbilt, *Comput. Mater. Sci.* **81**, 446 (2014) (link), for more information.

The GBRV pseudopotential library has been tested by comparing to all-electron LAPW+LO calculations performed with the WIEN2k code in a variety of chemical environments. The GBRV potential library has been found to produce lattice constants, bulk moduli, and magnetic moments which are of comparable or higher overall accuracy than other comprehensive pseudopotential libraries across a wide variety of bonding environments, while maintaining a low computational cost.

Please consult our paper (local preprint) for full details on our design criteria and testing procedure, and extra notes on the Abinit potentials and testing data.

While these potentials have been designed for high-throughput calculations, they should be of general use. Despite our relatively thorough testing, **we cannot guarantee that these potentials will be appropriate for every application**, but we provide testing data as well as the input files for use with the Vanderbilt Ultrasoft pseudopotential generator code, which can be used to modify the potentials to suit your needs. Please let us know if you improve on any of the potentials.

Kevin F. Garrity
Research Associate
NIST

Formerly Postdoc at Rutgers University
kgarrity@physics.rutgers.edu

Pseudopotential libraries
http://www.quantum-simulation.org/potentials/sg15_oncv/

quantum-simulation.org

Home

SG15 ONCV Potentials

The SG15 Optimized Norm-Conserving Vanderbilt (ONCV) pseudopotentials were generated using the code ONCVPSP (Optimized Norm-Conservinng Vanderbilt PSeudopotential) scalar-relativistic version 2.1.1, 03/26/2014 by D. R. Hamann. The code is available at www.mat-simresearch.com. and the procedure is described in

> D. R. Hamann, Phys. Rev. B 88, 085117 (2013)
> http://link.aps.org/doi/10.1103/PhysRevB.88.085117

The parameters of the SG15 potentials were optimized to reproduce the results of all-electron calculations with high accuracy, using the procedure described in

> M. Schlipf and F. Gygi, Computer Physics Communications **196**, 36 (2015).
> http://dx.doi.org/10.1016/j.cpc.2015.05.011.

License

The SG15 potentials are distributed under a Creative Commons Attribution-ShareAlike 4.0 license (CC BY-SA 4.0). See http://creativecommons.org/licenses/by-sa/4.0/

Download

The SG15 collection of ONCV pseudopotentials is available in UPF and XML formats.

- sg15_oncv_xml_2015-10-07.tar.gz SG15 ONCV potentials in XML format
- sg15_oncv_upf_2015-10-07.tar.gz SG15 ONCV potentials in UPF format

The XML format conforms to the quantum-simulation.org XML Schema specification http://www.quantum-simulation.org/schemas/species.xsd

Version numbers

Potential file names reflect their version number, starting with 1.0. As of 2015-10-20, some potentials have version number 1.1 after some defects were corrected. The downloadable files provided below only include the most recent version of each potential. The full collection including older versions is available as sg15_oncv_2015-10-07.tar.gz

Revision history

[2015-10-07]
Generated potentials for Hf, Ta, W without f electrons in valence. Updated full reference to the SG15 paper in potential files.
[2015-08-25]
Added reference to the SG15 paper in potential files.
[2015-05-20]
Updated potentials (version 1.1) for Ar, As, Cl, Cs, I, In, P, S, Sb, Se, Si, Sn, Te, Xe.
[2015-01-24]
Original distribution.

Quantum-ESPRESSO input file

```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
/
&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.    0.    0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```

$$n(\mathbf{r}) = \sum_{n\mathbf{k}} |\psi_{n\mathbf{k}}(\mathbf{r})|^2 \theta(\epsilon_n(\mathbf{k}) - \epsilon_F)$$

occupations = "smearing"
smearing = "gaussian" or mv, mp, fd
degauss = 0.01 in Ry (careful: the bands are printed in eV)

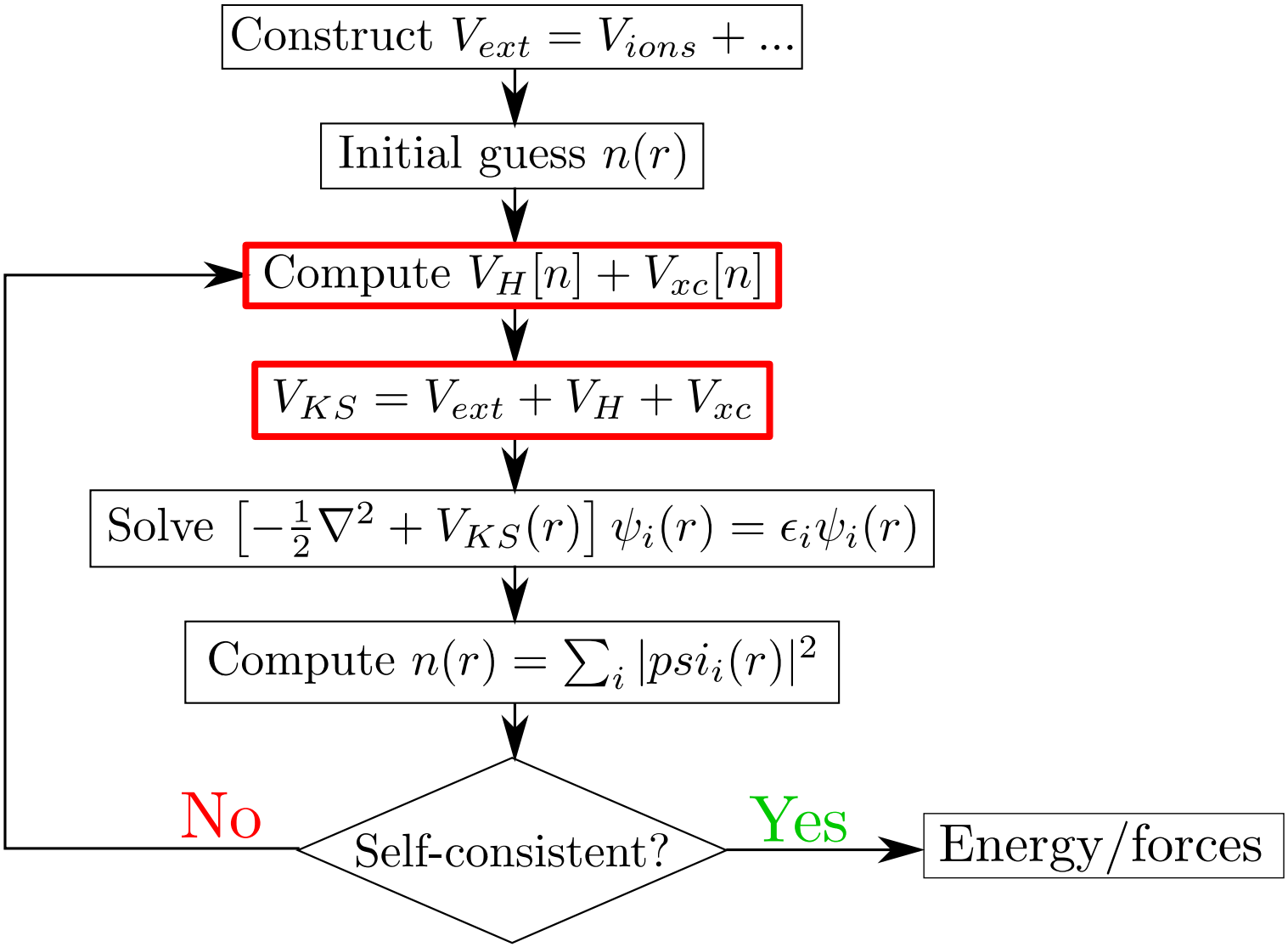
Smaller values of smearing are important for magnetic systems.

A small fictitious smearing can help convergence of molecules, small gap insulators

Some features not available for "metals" (either real or fake), i.e. dielectric constant, effective charges

nk1, nk2, nk3, shift1, shift2, shift3
shift can be 0 or 1

Iterative Solution of the Kohn-Sham Equations



Quantum-ESPRESSO input file

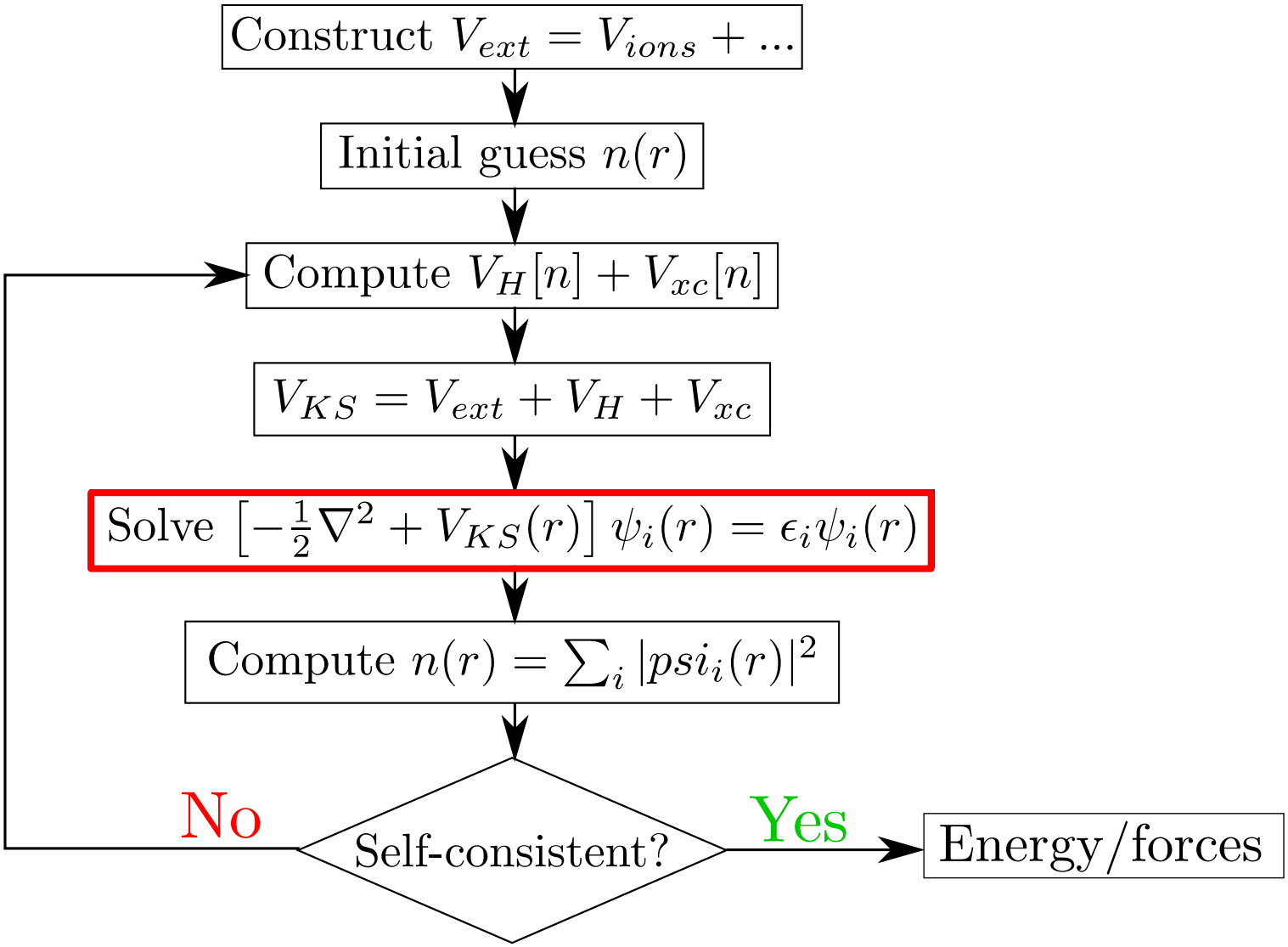
```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
/
&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.    0.    0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```

input_dft = "pbe0"
"b3lyp"
"rpbe"

Do not change the Functional unless you know what you are doing!

The default value is determined by the Pseudopotential!

Iterative Solution of the Kohn-Sham Equations



Quantum-ESPRESSO input file

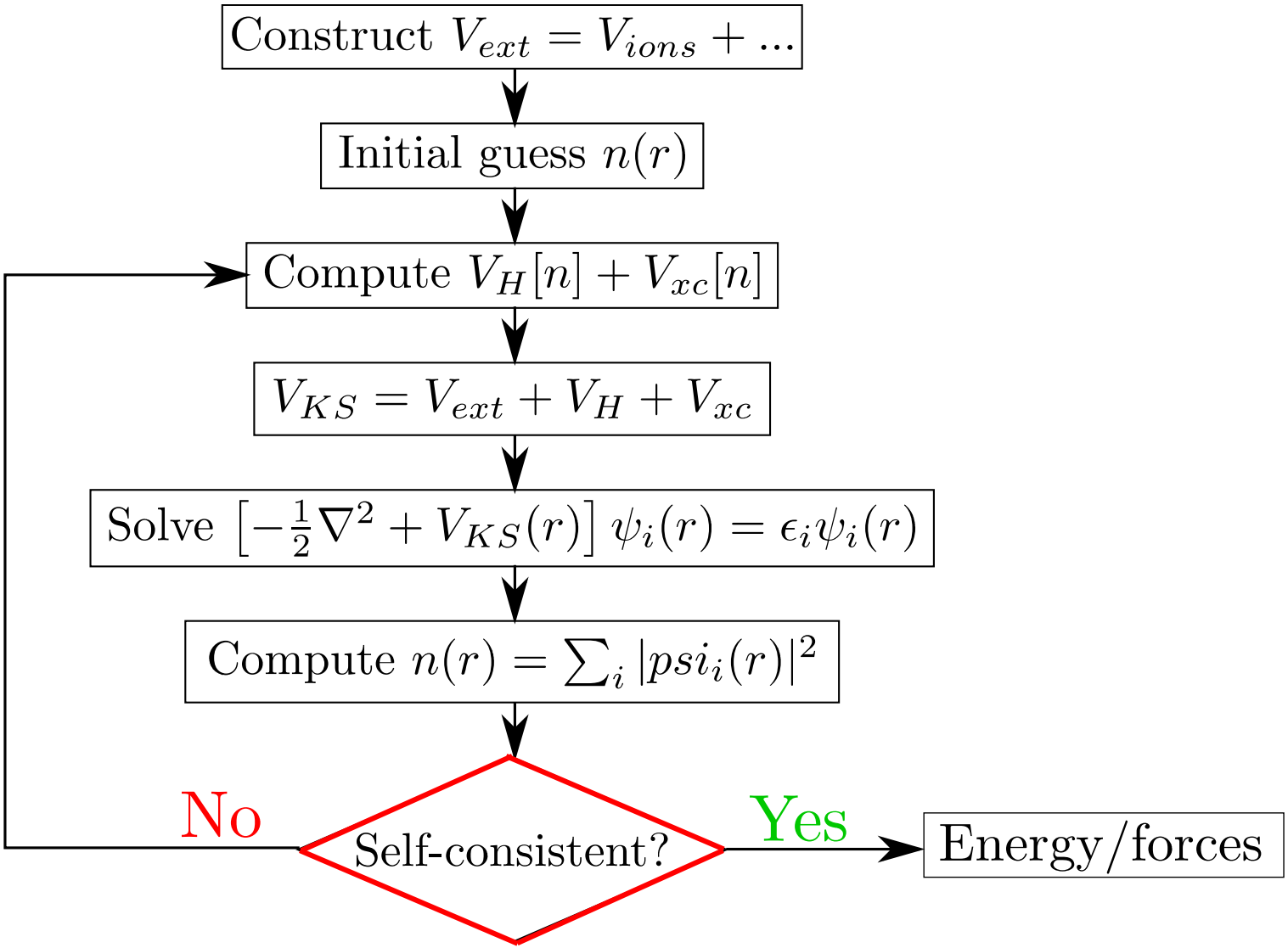
```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
/
&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.   0.   0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```

diagonalization = "david"

Very robust default algorithm, effective in parallel

Recourse to conjugate-gradient "cg" should never be needed: a fault in your input or bad pseudopotential is usually the cause of convergence problems.

Iterative Solution of the Kohn-Sham Equations

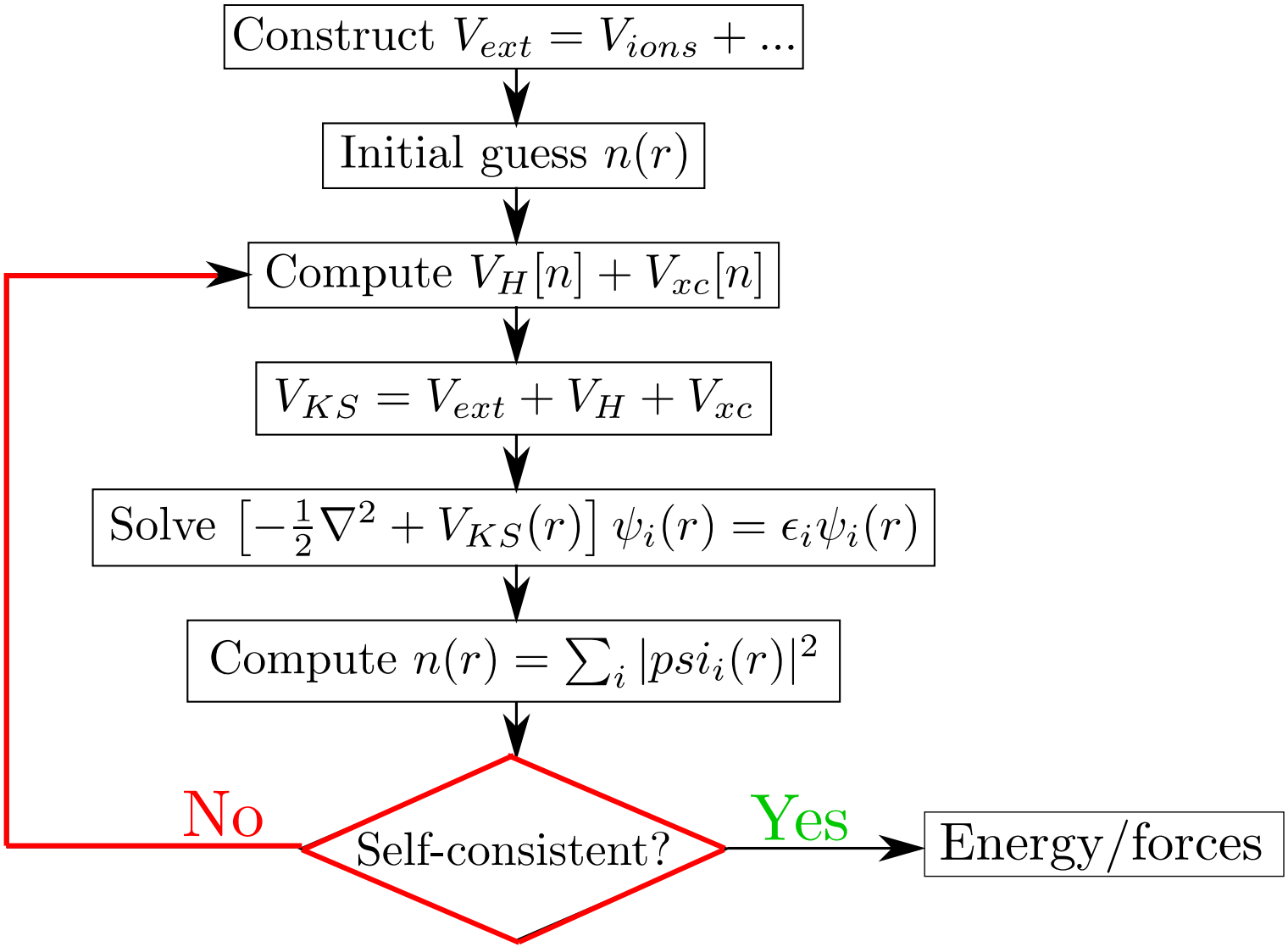


Quantum-ESPRESSO input file

```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
/
&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.   0.   0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```

conv_thr = 1.d-6 (DEFAULT)
1.d-10 (tight, good for phonons)

Iterative Solution of the Kohn-Sham Equations



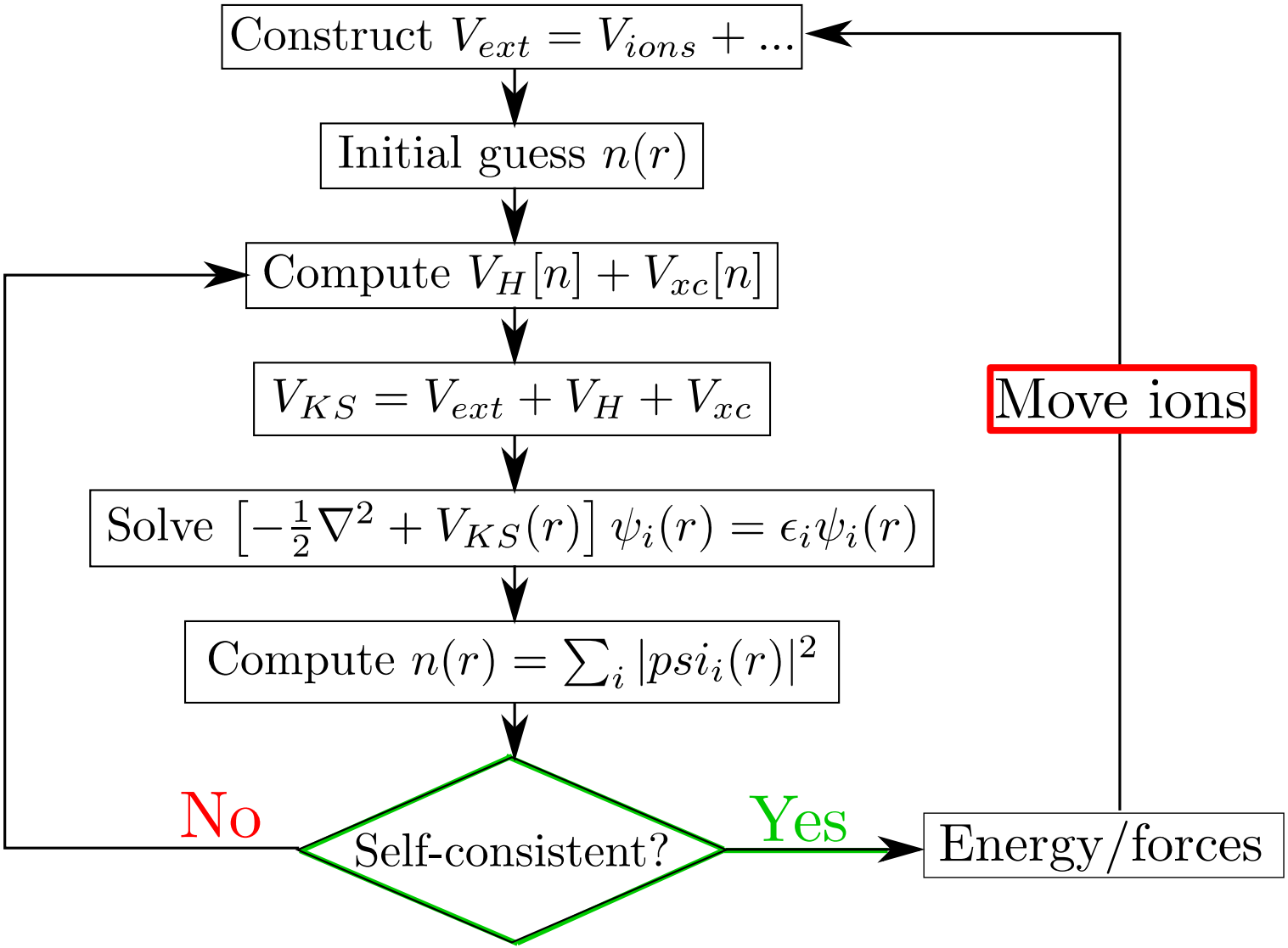
Quantum-ESPRESSO input file

```
&control
    calculation = "scf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
/
&electrons
    mixing_beta = 0.7
/
ATOMIC_SPECIES
 Si 28.086 Si.pz-rrkj.UPF
ATOMIC_POSITIONS alat
 Si 0.   0.   0.
 Si 0.25 0.25 0.25
K_POINTS automatic
 4 4 4  0 0 0
```

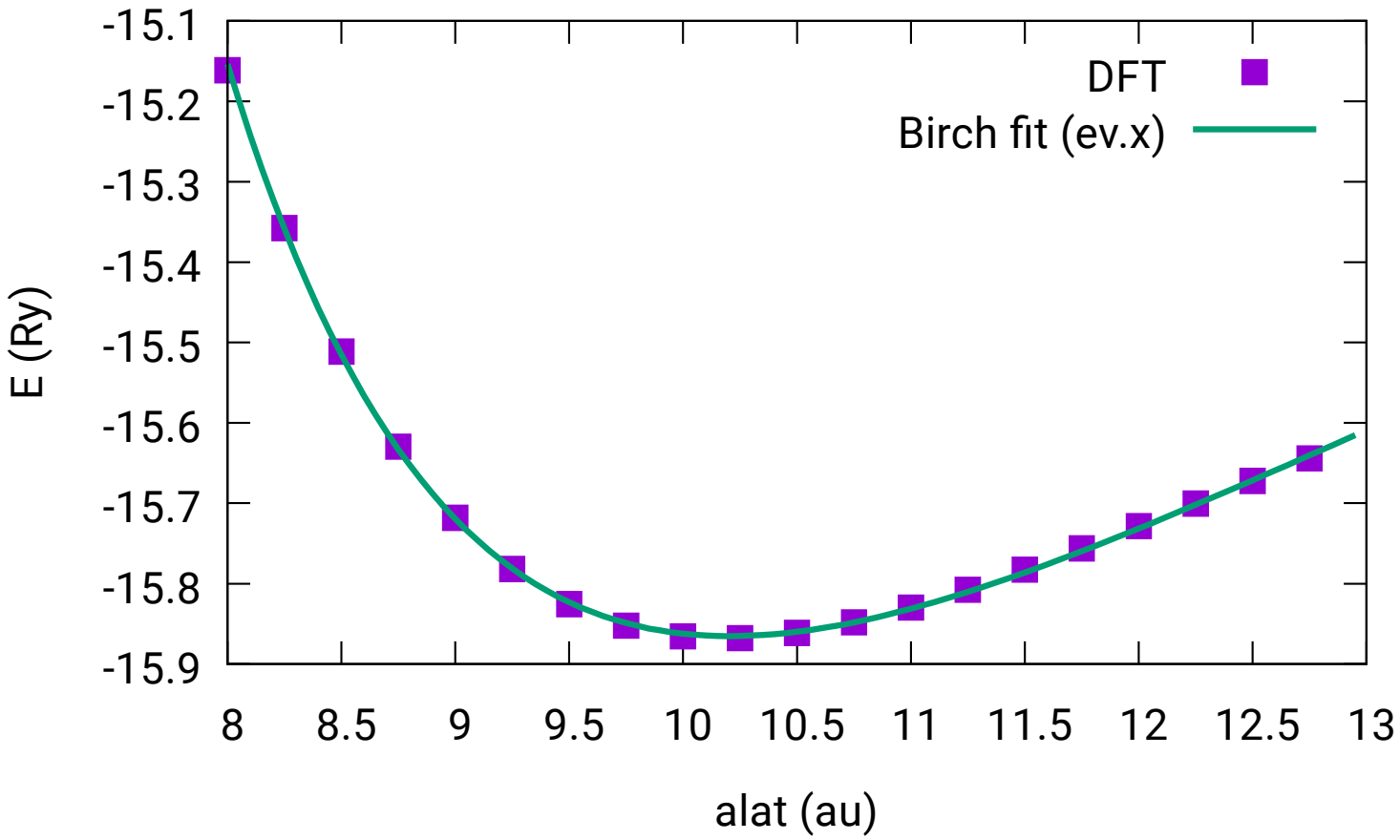
Mix new and old charge density using Broyden scheme

Lower the parameter for difficult systems (check also mixing_ndim)

Iterative Solution of the Kohn-Sham Equations



Equation of State



Series of DFT calculations, fitted with the ev.x utility

```
# equation of state: birch 1st order.  chisq = 0.8242D-05
# a0 = 10.2054 a.u., k0 =  869 kbar, dk0 =  4.08 d2k0 =  0.000 emin =  -15.86534
# a0 =  5.40044 Ang, k0 =  86.9 GPa,  V0 =   265.72 (a.u.)^3,  V0 =   39.38 A^3
```

Quantum-ESPRESSO input file

```
&control
    calculation = "relax"
    prefix = "silicon"
    outdir = "tmp"
    nstep = 50
    etot_conv_thr = 1.d-4
    forc_conv_thr = 1.d-3
/
...
&electrons
    conv_thr = 1.d-8
/
&ions
    ion_dynamics = "bfgs"
    upscale = 100
pot_extrapolation="atomic"
/
&cell
    press = 0.0
/
...
```

vc-relax, md, vc-md

pw.x can move the ions according to many different schemes: check the documentation and literature.

Consider Car-Parrinello

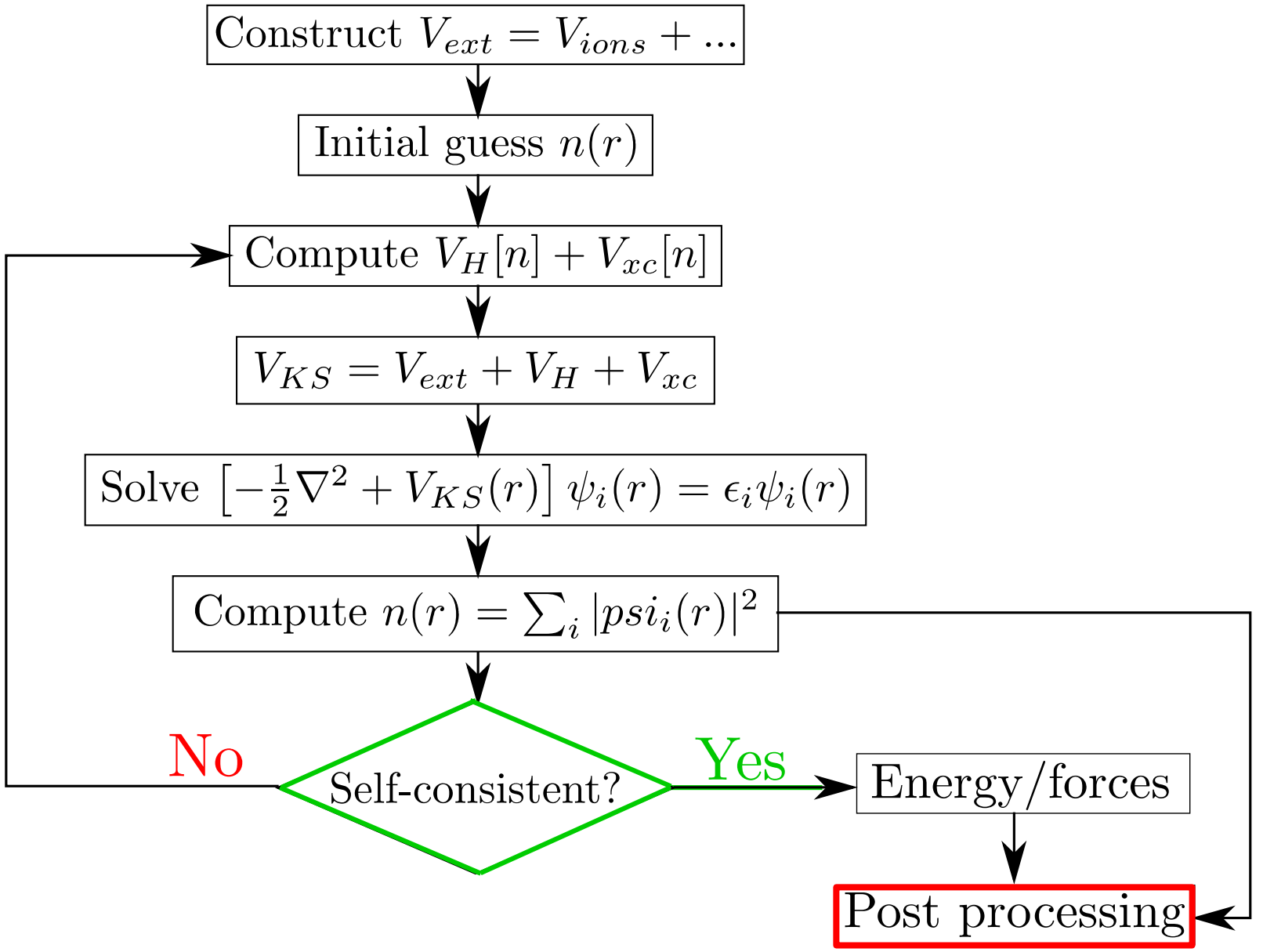
Move the atoms by hand!

damp, verlet, langevin, ...

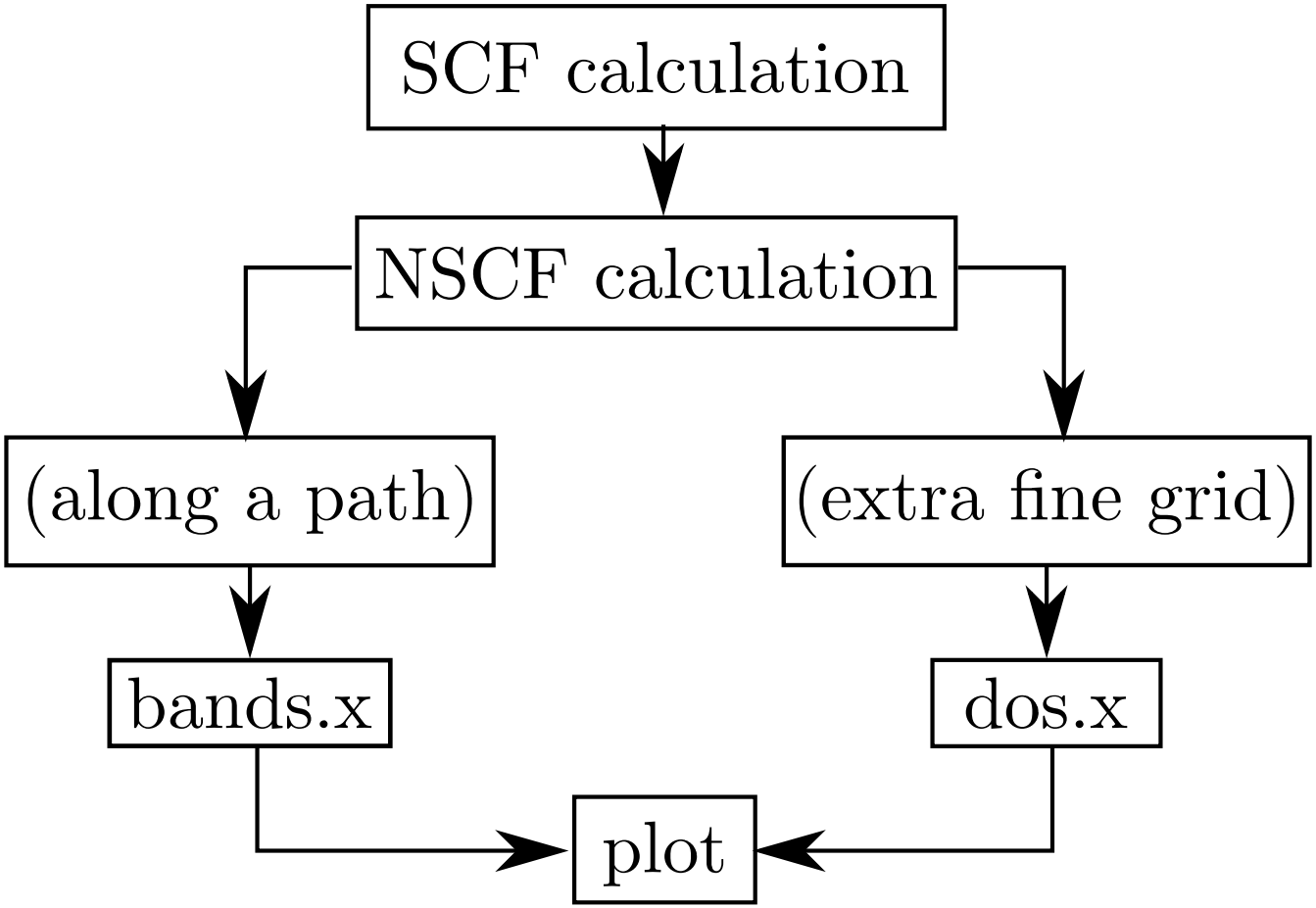
none, first_order, second_order

target pressure in kbar

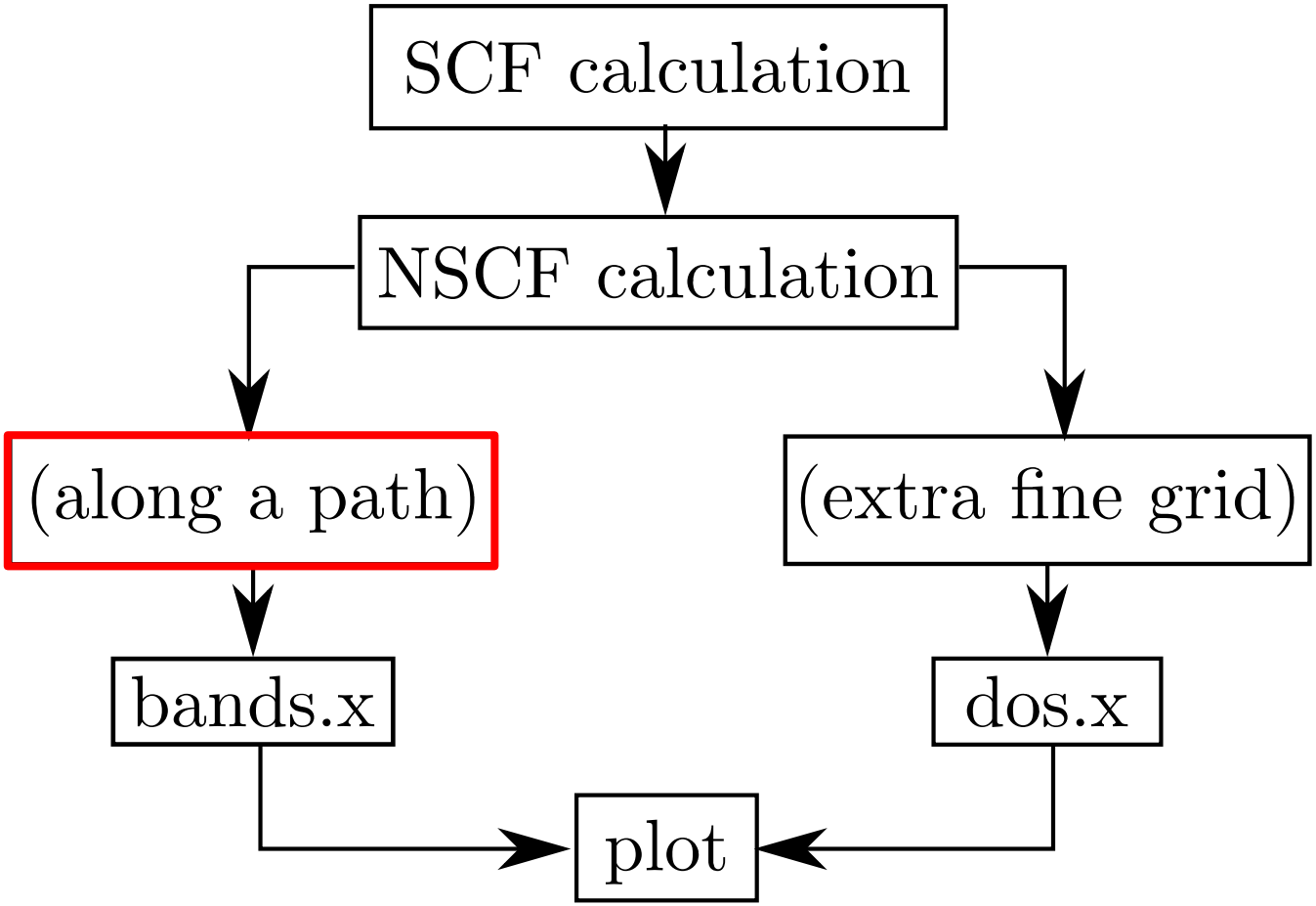
Iterative Solution of the Kohn-Sham Equations



Post-processing



Post-processing



Quantum-ESPRESSO input file

```
&control
    calculation = "bands"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
    nbnd = 20
/
...
K_POINTS tpiba_b
3
0.50 0.50 0.50 50
0.00 0.00 0.00 40
0.00 0.00 1.00 20
```

L
X
Γ

Non-self consistent calculation for a series of q-points
Fermi energy is not recomputed

DEFAULT : only valence bands are used
(a few more for metals)

Or set-up a path to compute the bands

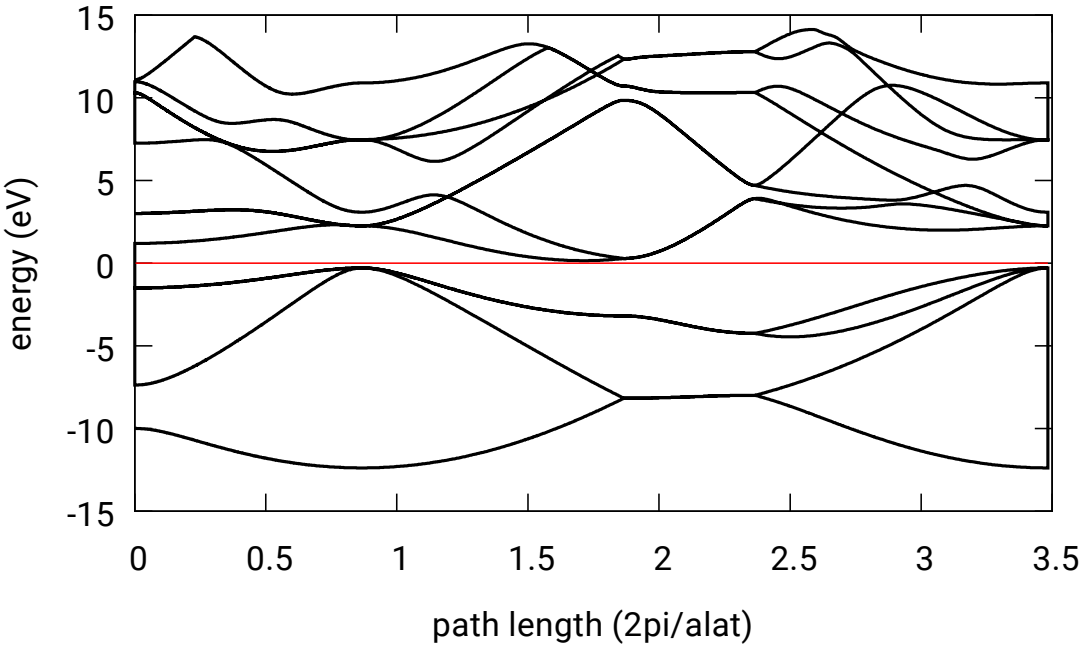
bands.x input file

```
&bands
  prefix = "silicon"
  outdir = "tmp/"
  filband= "siband.dat"

  lsym = .true.
  no_overlap = .true.
/
```

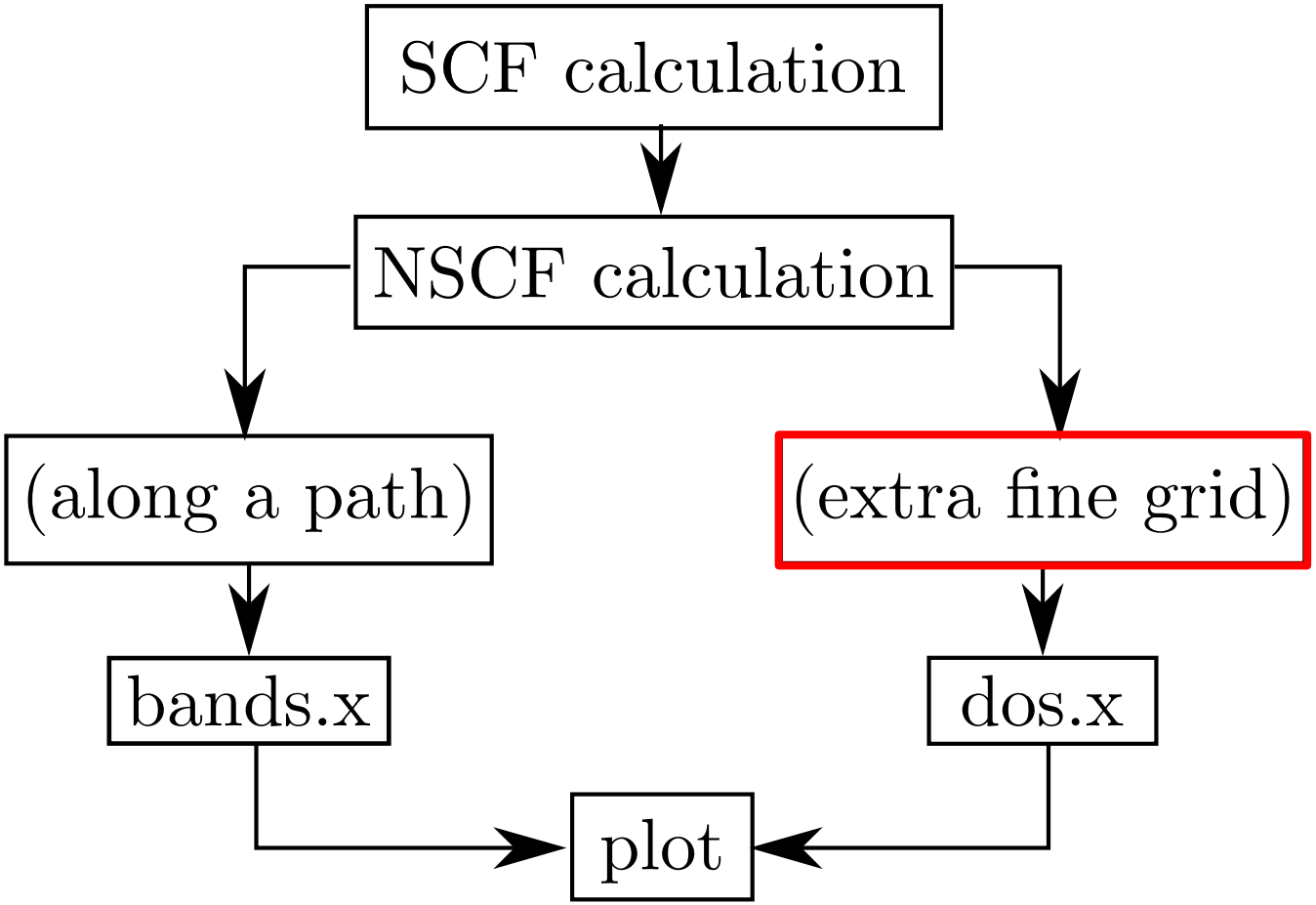
Many available options, depending on the kind of plot you want: see PP/Doc/INPUT_BANDS.txt

Can classify bands by symmetry or computing overlap between wavefunction at subsequent points



Output can be plot directly (file ".gnu") or further processed with plotbands.x

Post-processing



Quantum-ESPRESSO input file

```
&control
    calculation = "nscf"
    prefix = "silicon"
    outdir = "tmp"
/
&system
    ibrav = 2
    celldm(1) = 10.20
    nat = 2
    ntyp = 1
    ecutwfc = 16.0
    nbnd = 20
  occupation="tetrahedra"
/
...
K_POINTS automatic
16 16 16  0 0 0
```

Simple integration scheme without any free parameter, otherwise:

```
occupation= "smearing"
smearing  = "gaussian"
degauss   = 0.01
```

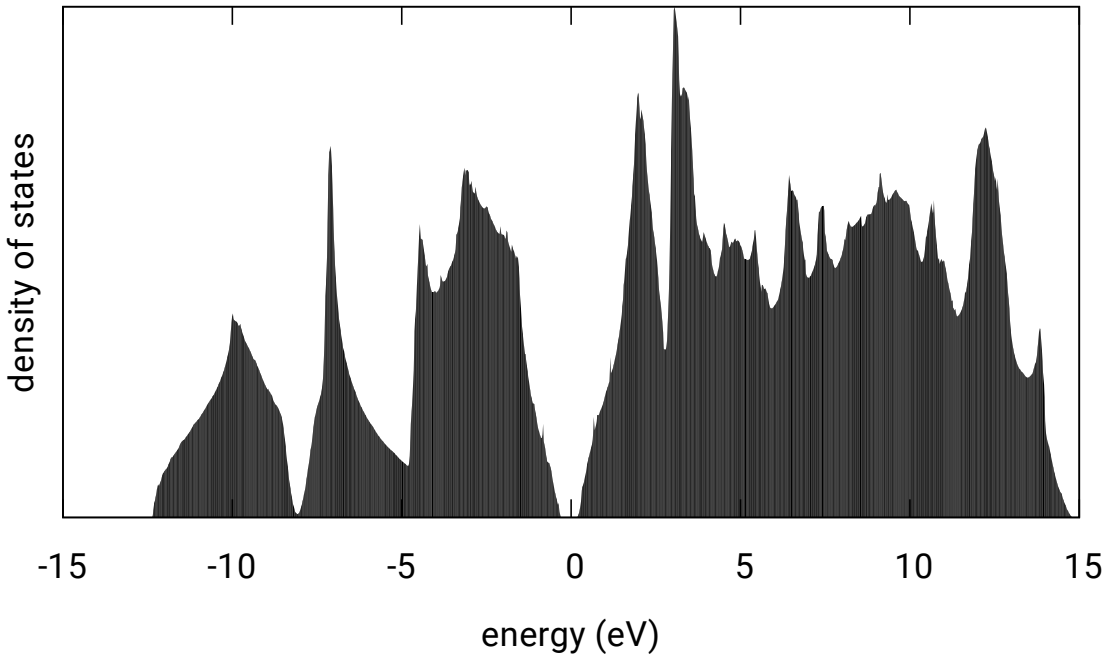
dos.x input file

```
&dos
   prefix = "silicon"
   outdir = "tmp/"
   fildos = "sidos.dat"

/
```

You can also change the kind and value of smearing used in pw.x, many more options

(see PP/Doc/INPUT_PP.txt)



Output can be plot directly (e.g. with gnuplot)

Tips

- Read the instructions
  - http://www.quantum-espresso.org/users-manual/
  - www.quantum-espresso.org/tutorials/
- Do not expect setting up a calculation to be fast and easy
- Ask for help:
  - http://www.qe-forge.org/mailman/listinfo/pw_forum

Hands-on session starting at 1PM
Computer Room 119, Atrium Building

Slides material: Simone Piccinin, Paolo Giannozzi, Stefano de Gironcoli, …