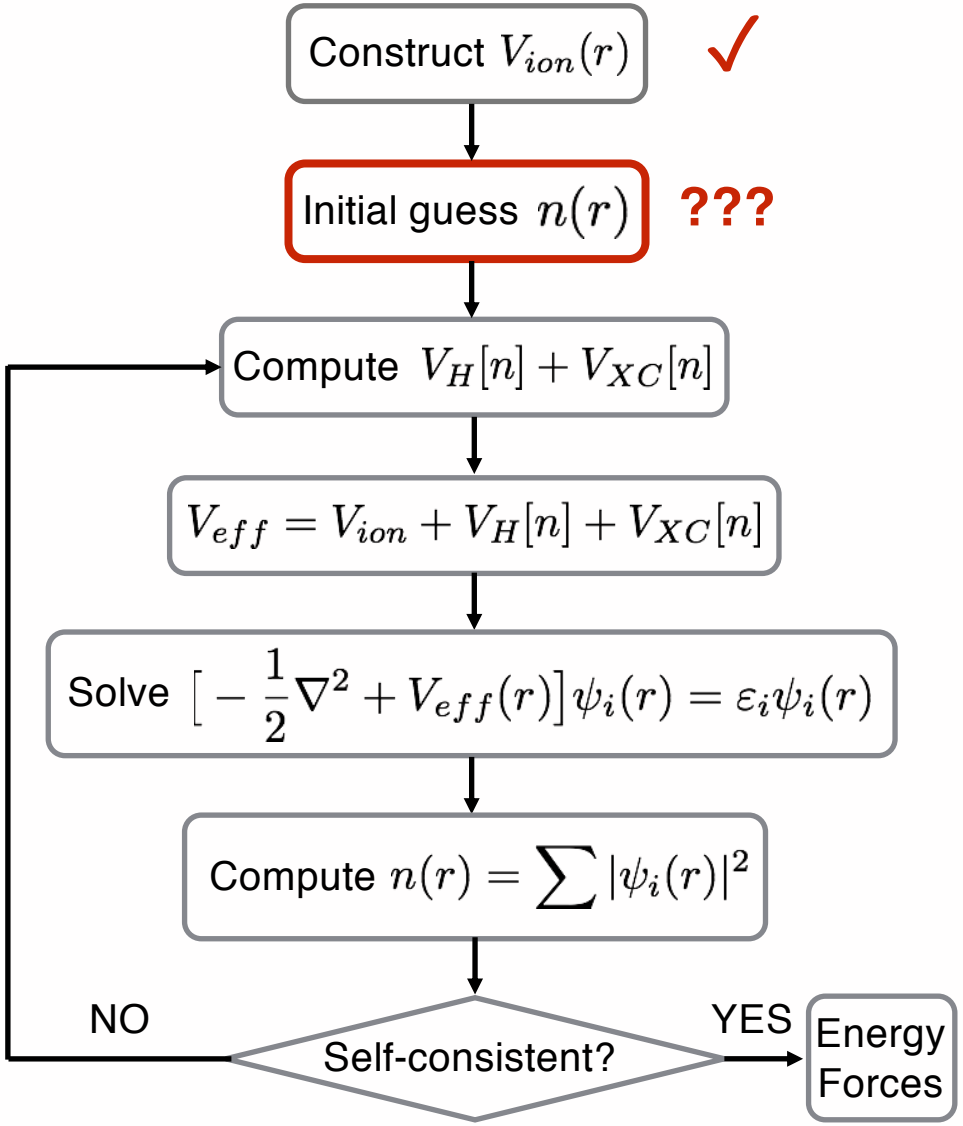
PART 5

MATERIAL DESIGN

QUANTUM ESPRESSO SCF CALCULATION

HANDS-ON #1

Initial n(r)

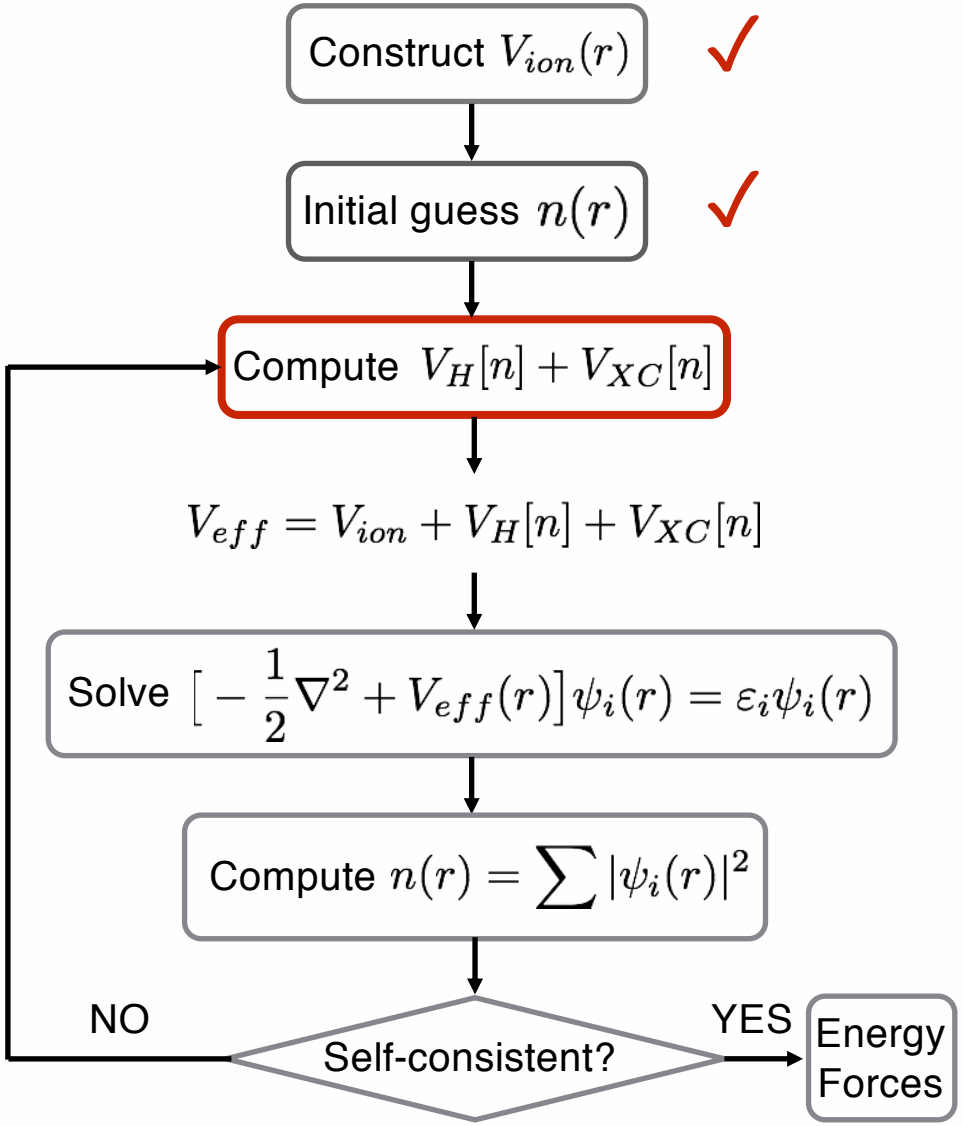

Construct $V_{ion}(r)$
✓
Initial guess $n(r)$
???
Compute $V_H[n] + V_{XC}[n]$
$V_{eff} = V_{ion} + V_H[n] + V_{XC}[n]$
Solve $\left[-\frac{1}{2}\nabla^2 + V_{eff}(r)\right]\psi_i(r) = \varepsilon_i\psi_i(r)$
Compute $n(r) = \sum |\psi_i(r)|^2$
NO
Self-consistent?
YES
Energy
Forces

Initial electron density n(r)

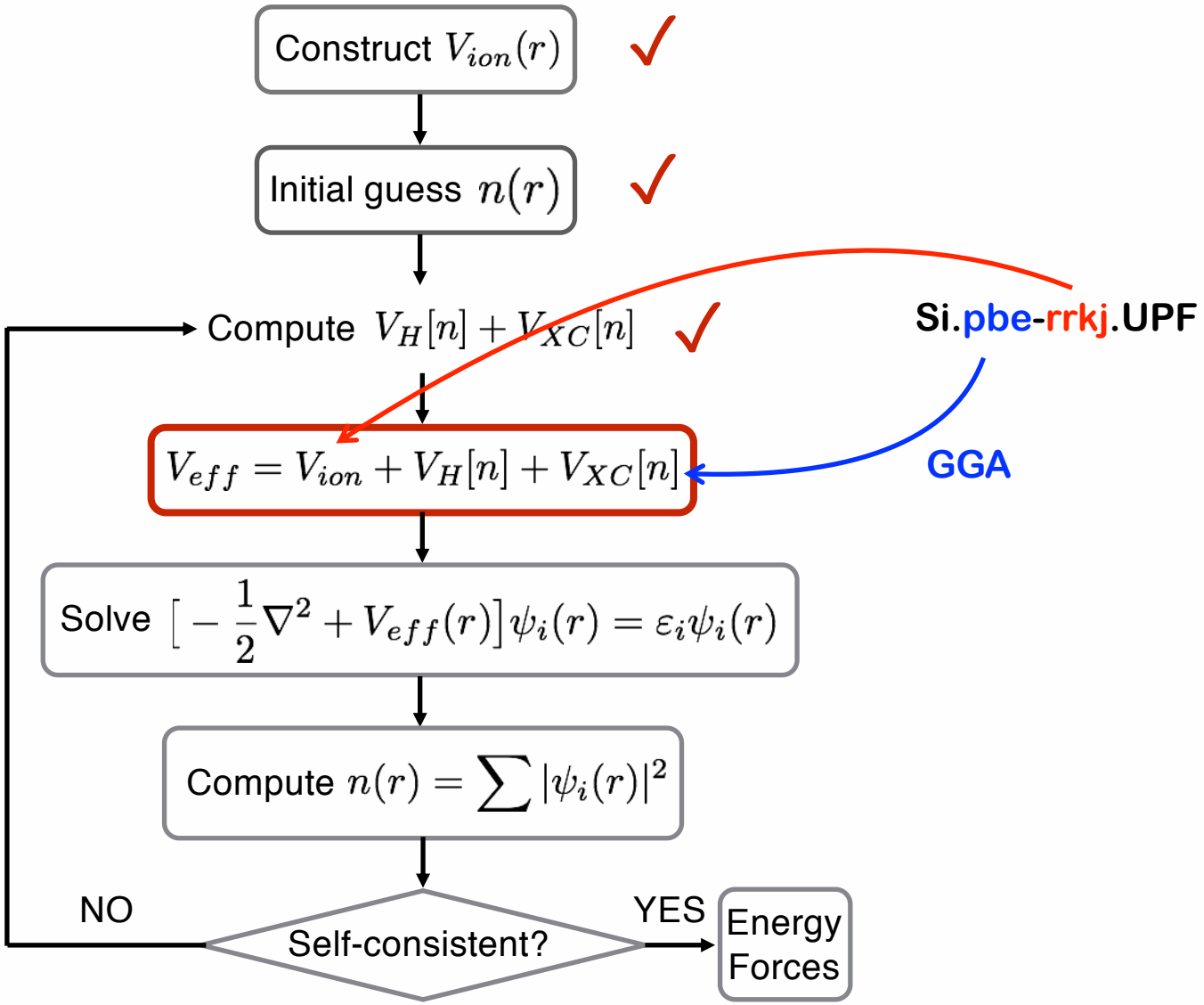
```
&CONTROL
 calculation='scf',
 restart_mode='from_scratch',
 prefix='si',
 pseudo_dir='../pseudo/',
 outdir='../tmp/',
/
&SYSTEM
 ibrav=2,
 celldm(1)=10.2625,
 nat=2,
 ntyp=1,
 ecutwfc=60.0,
 ecutrho=720.0,
/
&ELECTRONS
 mixing_beta=0.7,
 conv_thr=1d-8,
/
ATOMIC_SPECIES
 Si 28.0855 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si  0.00  0.00  0.00
Si  0.25  0.25  0.25
K_POINTS automatic
4 4 4 1 1 1
```

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

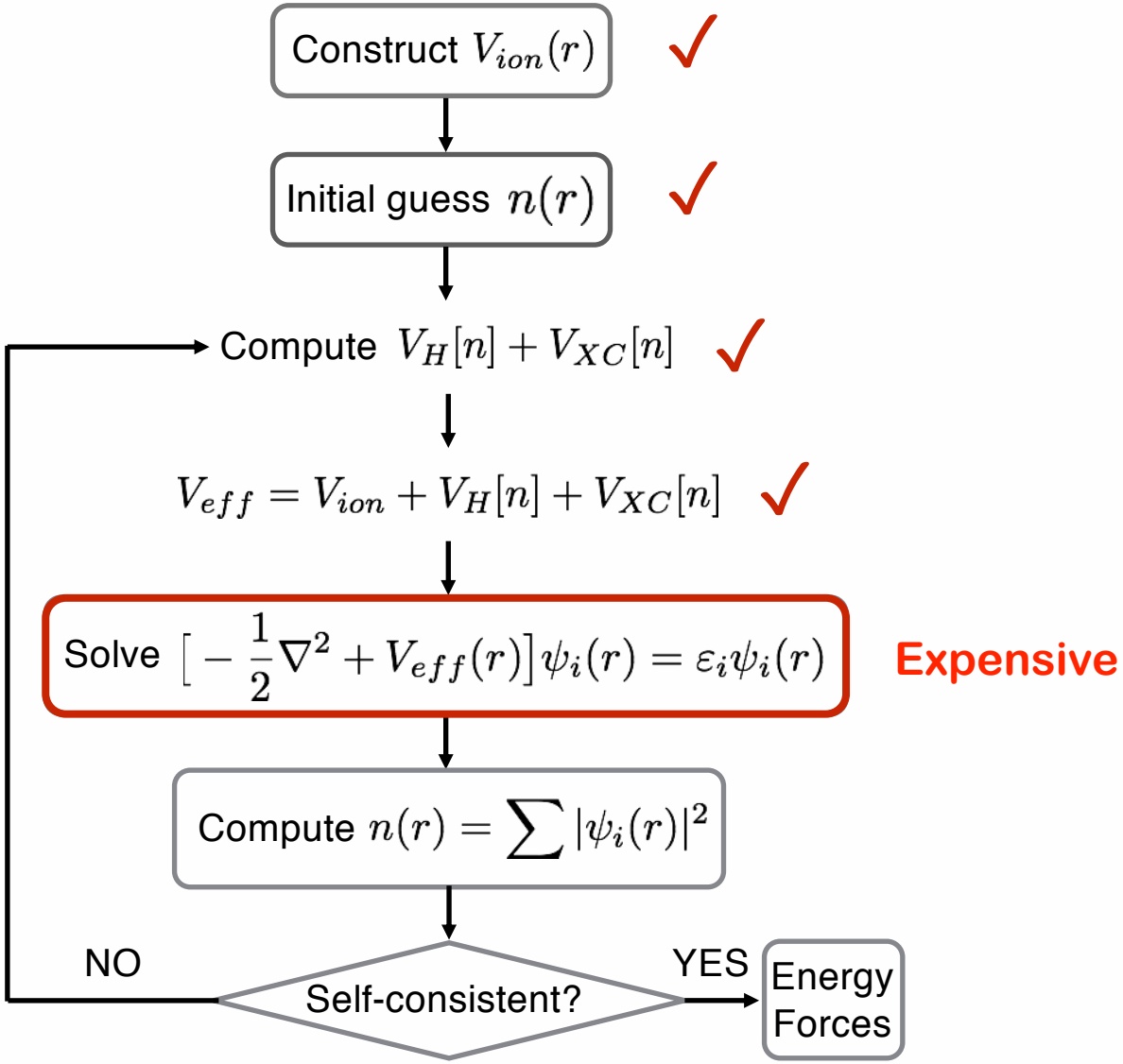
QE run


Construct $V_{ion}(r)$
Initial guess $n(r)$
Compute $V_H[n] + V_{XC}[n]$
$V_{eff} = V_{ion} + V_H[n] + V_{XC}[n]$
Solve $\left[-\frac{1}{2}\nabla^2 + V_{eff}(r)\right]\psi_i(r) = \varepsilon_i\psi_i(r)$
Compute $n(r) = \sum |\psi_i(r)|^2$
Self-consistent?
NO
YES
Energy
Forces

QE run


Construct $V_{ion}(r)$
Initial guess $n(r)$
Compute $V_H[n] + V_{XC}[n]$
$V_{eff} = V_{ion} + V_H[n] + V_{XC}[n]$
Solve $\left[-\frac{1}{2}\nabla^2 + V_{eff}(r)\right]\psi_i(r) = \varepsilon_i\psi_i(r)$
Compute $n(r) = \sum |\psi_i(r)|^2$
Self-consistent?
NO
YES
Energy
Forces
Si.pbe-rrkj.UPF
GGA

QE run



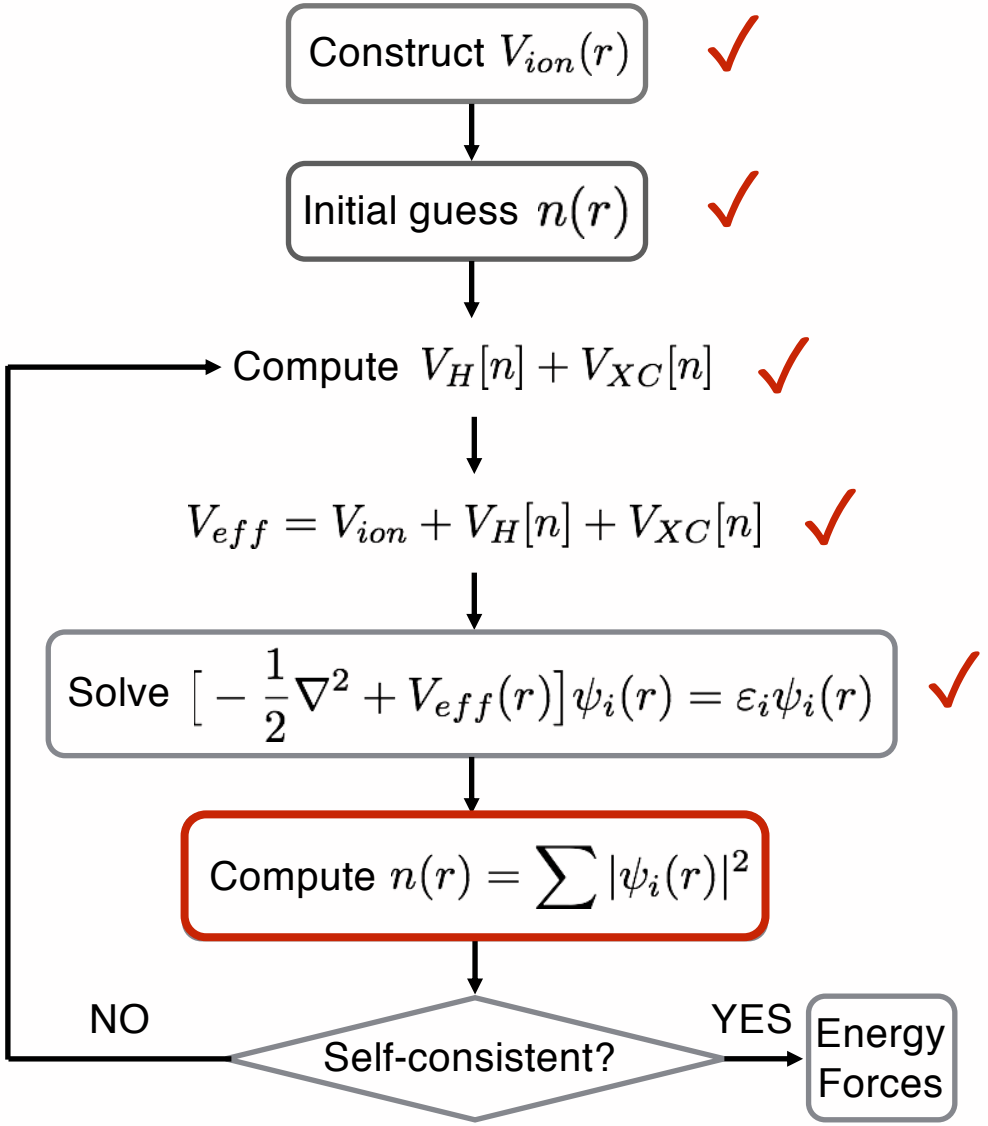
Expensive

Solve wave equation

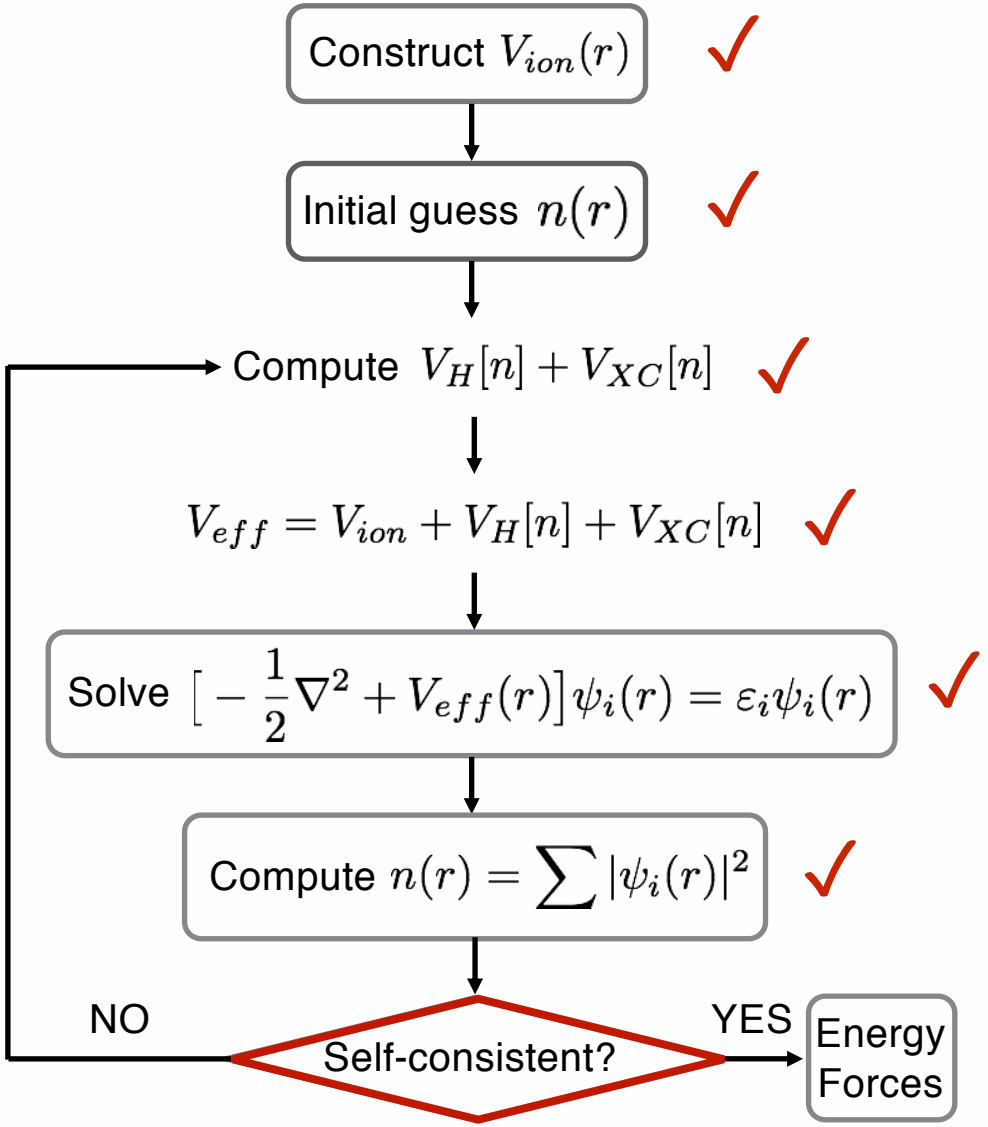
```
&CONTROL
 calculation='scf',
 restart_mode='from_scratch',
 prefix='si',
 pseudo_dir='../pseudo/',
 outdir='../tmp/',
/
&SYSTEM
 ibrav=2,
 celldm(1)=10.2625,
 nat=2,
 ntyp=1,
 ecutwfc=60.0,
 ecutrho=720.0,
/
&ELECTRONS
 mixing_beta=0.7,
 conv_thr=1d-8,
/
ATOMIC_SPECIES
 Si 28.0855 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si  0.00  0.00  0.00
Si  0.25  0.25  0.25
K_POINTS automatic
4 4 4 1 1 1
```

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

QE run


Construct $V_{ion}(r)$
Initial guess $n(r)$
Compute $V_H[n] + V_{XC}[n]$
$V_{eff} = V_{ion} + V_H[n] + V_{XC}[n]$
Solve $\left[-\frac{1}{2}\nabla^2 + V_{eff}(r)\right]\psi_i(r) = \varepsilon_i\psi_i(r)$
Compute $n(r) = \sum |\psi_i(r)|^2$
Self-consistent?
NO
YES
Energy
Forces

SCF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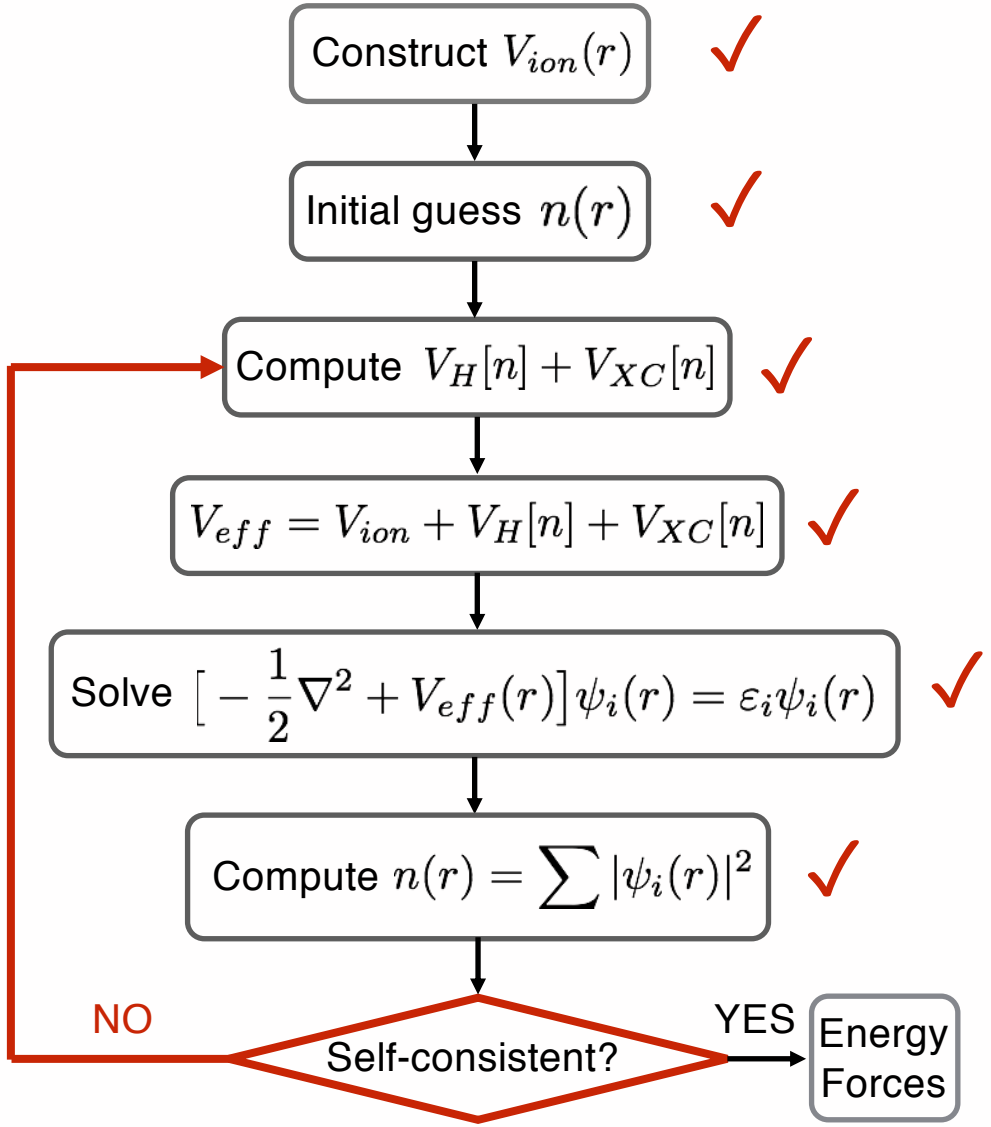
Initial guess $n(r)$
Compute $V_H[n] + V_{XC}[n]$
$V_{eff} = V_{ion} + V_H[n] + V_{XC}[n]$
Solve $\left[-\frac{1}{2}\nabla^2 + V_{eff}(r)\right]\psi_i(r) = \varepsilon_i\psi_i(r)$
Compute $n(r) = \sum |\psi_i(r)|^2$
Self-consistent?
NO
YES
Energy
Forces

Self-consistency

```
&CONTROL
 calculation='scf',
 restart_mode='from_scratch',
 prefix='si',
 pseudo_dir='../pseudo/',
 outdir='../tmp/',
/
&SYSTEM
 ibrav=2,
 celldm(1)=10.2625,
 nat=2,
 ntyp=1,
 ecutwfc=60.0,
 ecutrho=720.0,
/
&ELECTRONS
 mixing_beta=0.7,
 conv_thr=1d-8,
/
ATOMIC_SPECIES
 Si 28.0855 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si  0.00  0.00  0.00
Si  0.25  0.25  0.25
K_POINTS automatic
4 4 4 1 1 1
```

Convergence threshold for self-consistency:
estimated energy error > conv_thr (NO)
or energy error < conv_thr (YES)

SCF

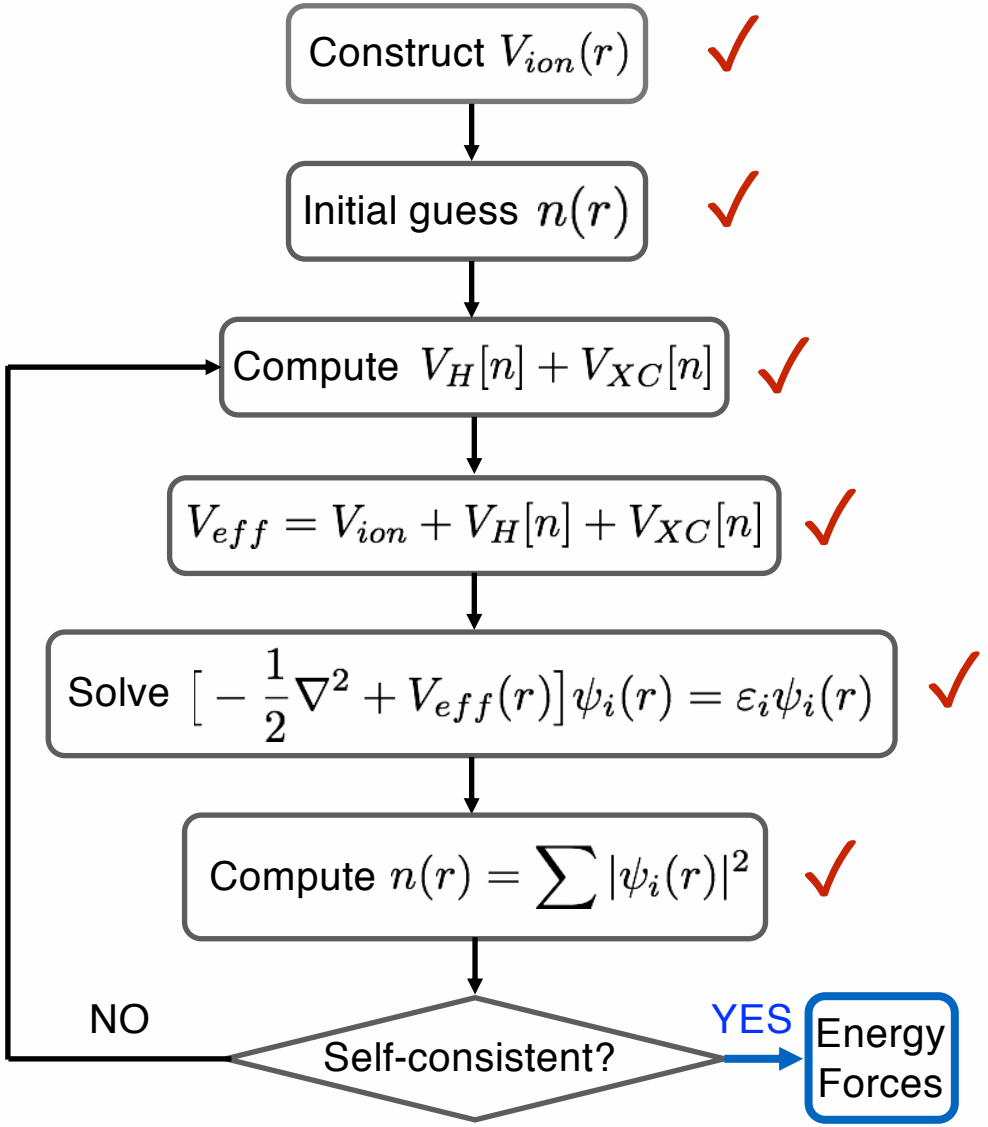

Construct $V_{ion}(r)$
Initial guess $n(r)$
Compute $V_H[n] + V_{XC}[n]$
$V_{eff} = V_{ion} + V_H[n] + V_{XC}[n]$
Solve $\left[-\frac{1}{2}\nabla^2 + V_{eff}(r)\right]\psi_i(r) = \varepsilon_i\psi_i(r)$
Compute $n(r) = \sum |\psi_i(r)|^2$
Self-consistent?
NO
YES
Energy
Forces

new n(r)

```
&CONTROL
 calculation='scf',
 restart_mode='from_scratch',
 prefix='si',
 pseudo_dir='../pseudo/',
 outdir='../tmp/',
/
&SYSTEM
 ibrav=2,
 celldm(1)=10.2625,
 nat=2,
 ntyp=1,
 ecutwfc=60.0,
 ecutrho=720.0,
/
&ELECTRONS
 mixing_beta=0.7,
 conv_thr=1d-8,
/
ATOMIC_SPECIES
 Si 28.0855 Si.pbe-rrkj.UPF
ATOMIC_POSITIONS (alat)
Si  0.00  0.00  0.00
Si  0.25  0.25  0.25
K_POINTS automatic
4 4 4 1 1 1
```

Mix new and old density:
0.7 = 70% of the new density and 30% of old density at first step

QE run


Construct $V_{ion}(r)$
Initial guess $n(r)$
Compute $V_H[n] + V_{XC}[n]$
$V_{eff} = V_{ion} + V_H[n] + V_{XC}[n]$
Solve $\left[-\frac{1}{2}\nabla^2 + V_{eff}(r)\right]\psi_i(r) = \varepsilon_i\psi_i(r)$
Compute $n(r) = \sum |\psi_i(r)|^2$
Self-consistent?
NO
YES
Energy
Forces

Total energy

command:

```
$ pw.x <Si.scf.in> Si.scf.out &
$ grep ! Si.scf.out
```

```
     highest occupied level (ev):     5.9399

!    total energy              =     -15.74122935 Ry
     Harris-Foulkes estimate   =     -15.74122935 Ry
     estimated scf accuracy    <          8.8E-09 Ry

     The total energy is the sum of the following terms:

     one-electron contribution =       4.77318714 Ry
     hartree contribution      =       1.09508506 Ry
     xc contribution           =      -4.81266477 Ry
     ewald contribution        =     -16.79683678 Ry

     convergence has been achieved in   6 iterations

     Writing output data file si.save

     init_run     :      0.59s CPU      0.88s WALL (       1 calls)
     electrons    :      1.24s CPU      1.52s WALL (       1 calls)

     Called by init_run:
     wfcinit      :      0.08s CPU      0.22s WALL (       1 calls)
     potinit      :      0.06s CPU      0.07s WALL (       1 calls)
```