Converge siesta calculations

Mesh, k-points and SCF convergence

Catalina Coll

3th October 2023

MAX DRIVING THE EXASCALE TRANSITION
cecam Centre Européen de Calcul Atomique et Moléculaire
BSC Barcelona Supercomputing Center Centro Nacional de Supercomputación
ICN2 Institut Català de Nanociència i Nanotecnologia

Quality/accuracy/precision

Monday 2nd October	
12:30–12:45	Introductory remarks
12:45–13:30	General Siesta Theory (Prof. José Soler, UAM)
13:30–13:55	Pseudopotentials (Dr. Alberto García, ICMAB-CSIC)
13:55–14:10	Break
14:10–16:00	A first contact with SIESTA: inputs, execution and outputs (Dr. Federico Pedron, ICN2)
16:00–16:15	Break
16:15–17:15	Basis sets in SIESTA (Dr. Miguel Pruneda, CINN-CSIC)
17:15–17:30	Discussion and feedback
Tuesday 3rd October	
12:30–14:30	Basis set optimization (Dr. Federico Pedron, ICN2)
14:30–14:45	Break
14:45–16:15	K-points, mesh, and SCF convergence (Dr. Catalina Coll, ICN2)

System geometry

Pseudo potential

Real space grid

SCF convergence parameters

Basis Set

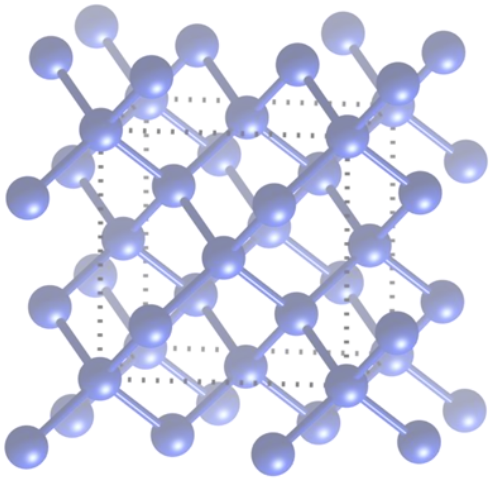
Reciprocal space grid

Sampling

Sampling

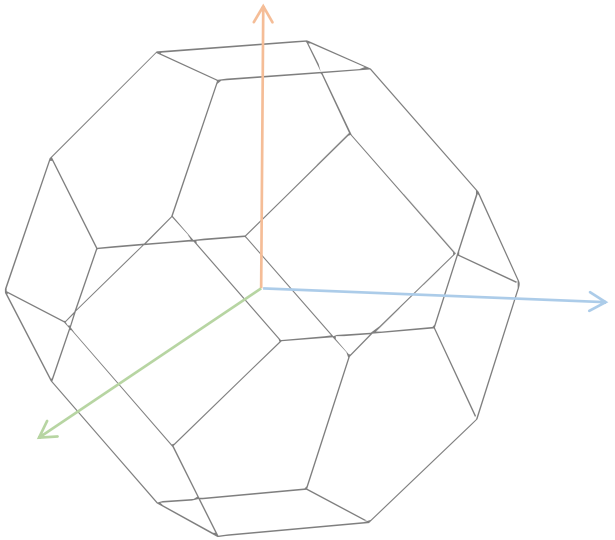
Real space

- **Potentials**
- **Densities**
- **Basis**

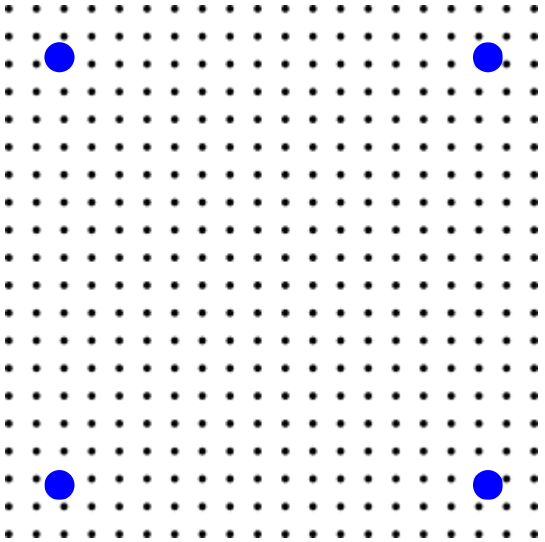


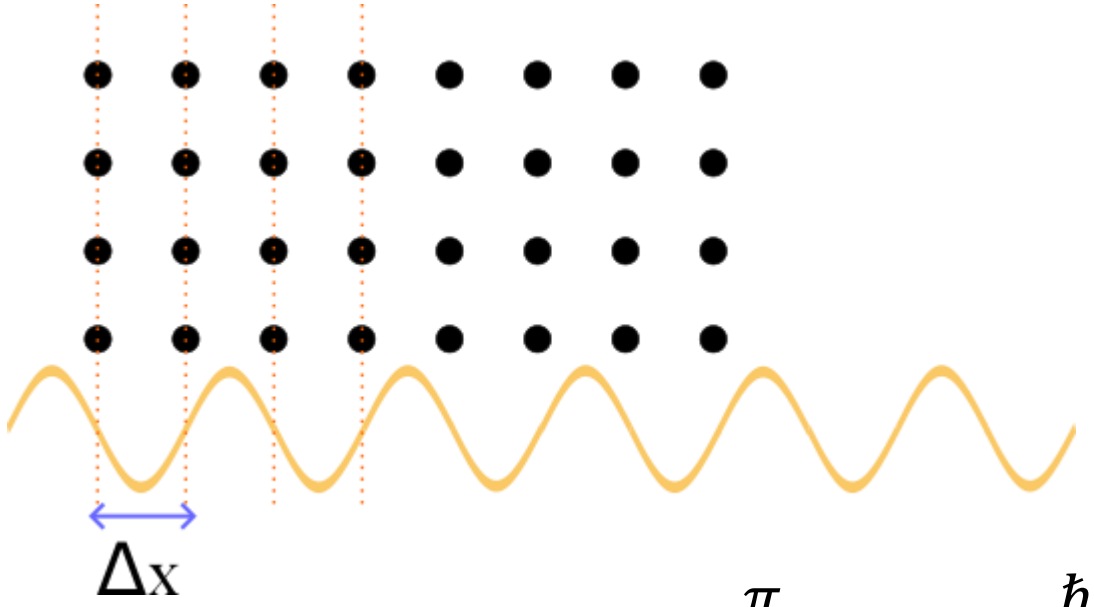
Reciprocal space

- **Density of states**
- **Bandstructure**



Real space grid





$$\Delta x \rightarrow k_c = \frac{\pi}{\Delta x} \rightarrow E_c = \frac{\hbar^2 k_c^2}{2m_e}$$

Fineness ↔ Maxim energy avoiding aliasing

$$\Delta x \leftrightarrow E_c$$ MeshCutoff

Energy units (Ry)

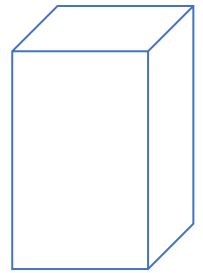
Real space grid: MeshCutoff

- What is it set by the user?
  - Mesh.Cutoff 300 Ry (default)

```
Mesh.Cutoff 100 Ry
```

- What is set by siesta?
  - MESH = 18 x 18 x 30 = 9720
  - Mesh cutoff (required, used) = 100.000 101.039 Ry

Input structure → Lattice vectors

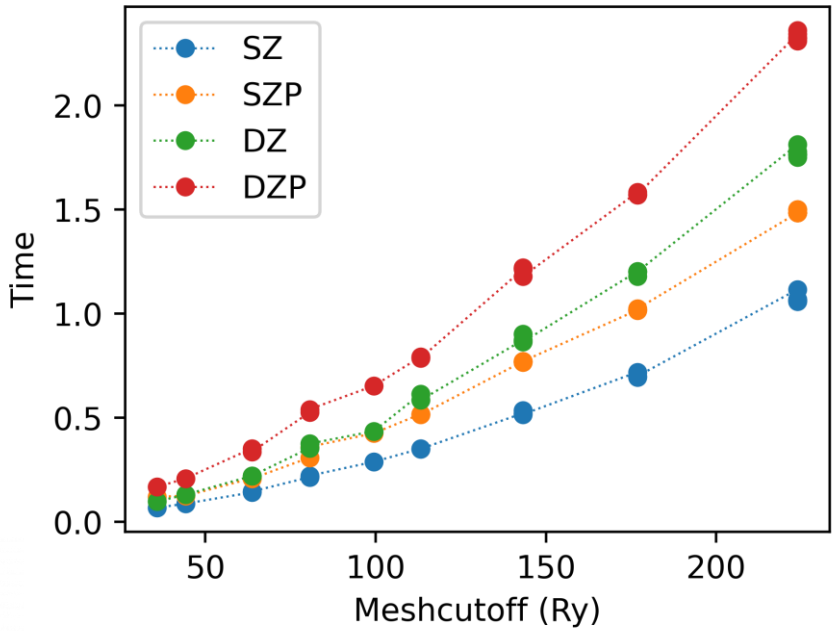


- How can one decide the good value?
  - Minimize the total energy.
  - Total force to zero.
  - Reasonable time (relatively small systems)

Real space grid: MeshCutoff

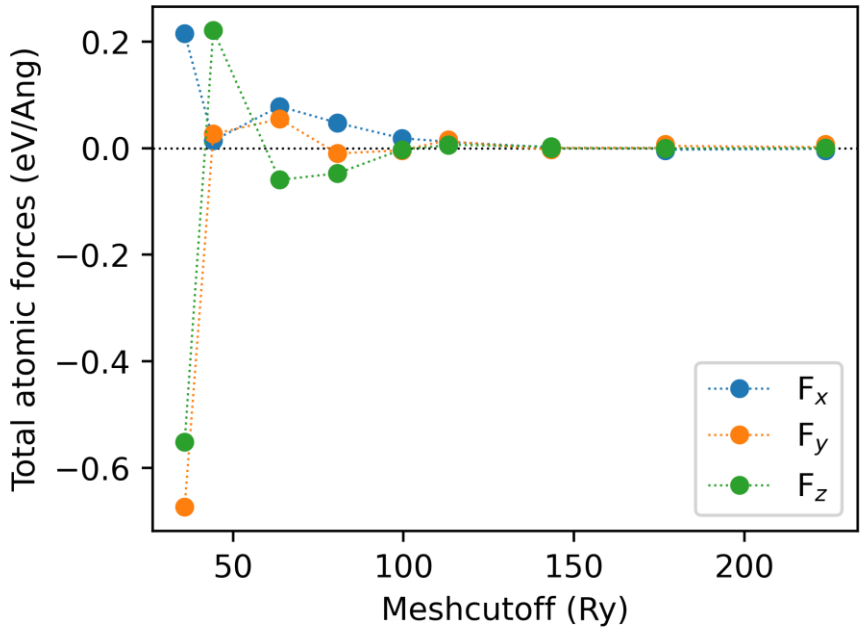
Time

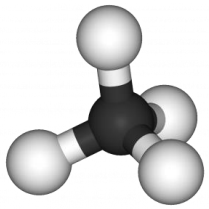
`TIMES file`



Force

`siesta: Atomic forces (eV/Ang):`



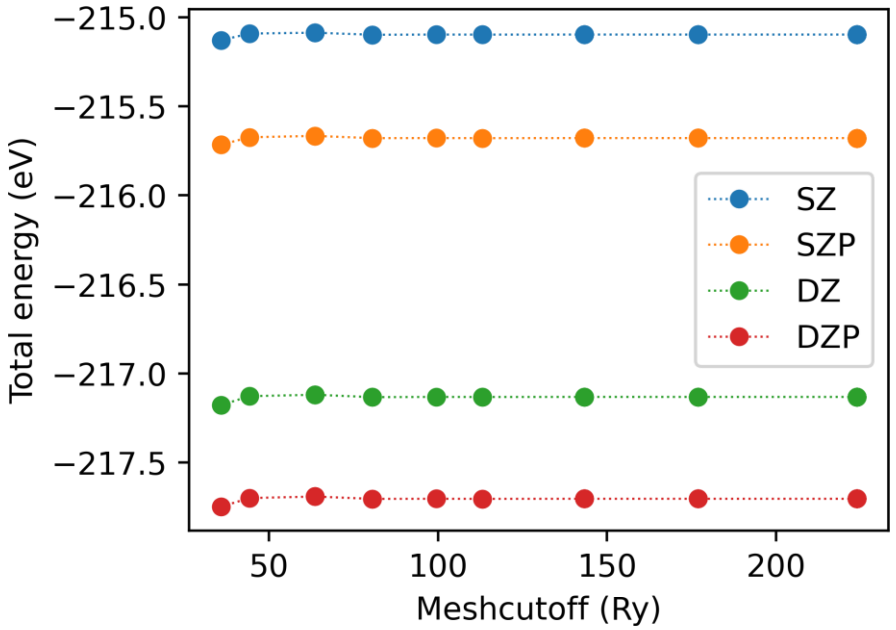


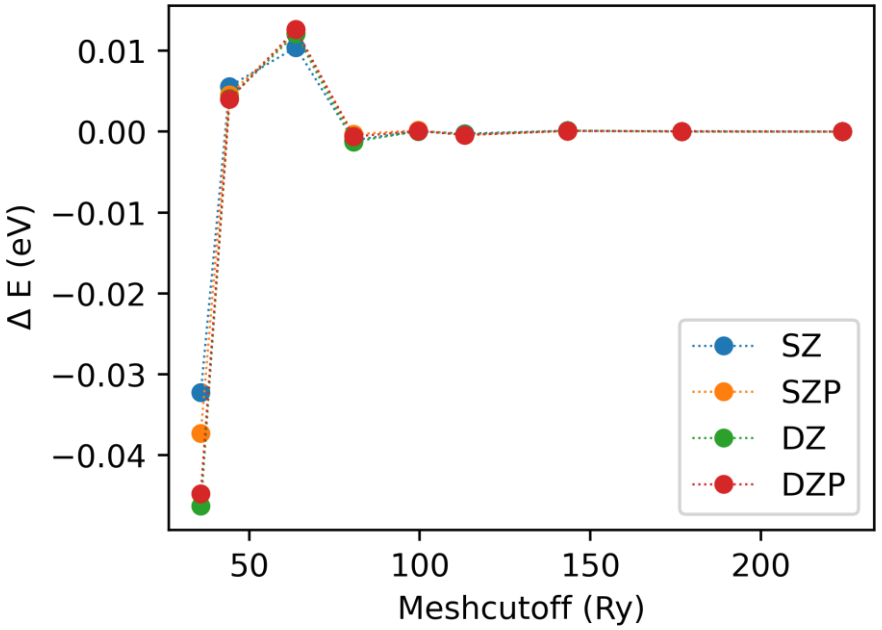
Results for methane (CH4)

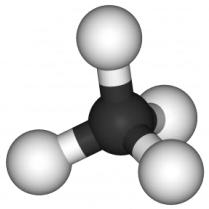
Real space grid: MeshCutoff

Energy

```
siesta: Final energy (eV):
```

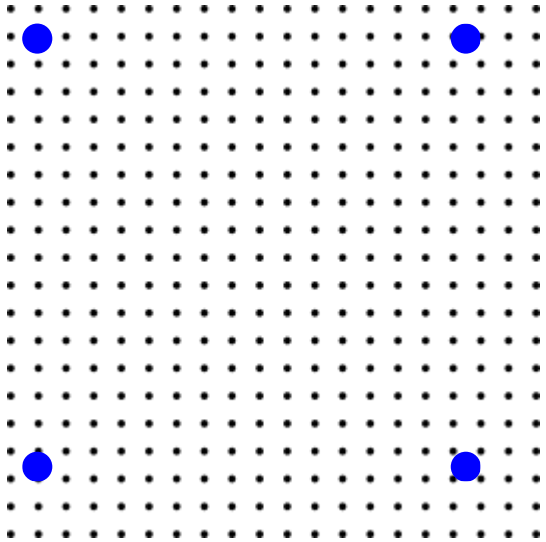




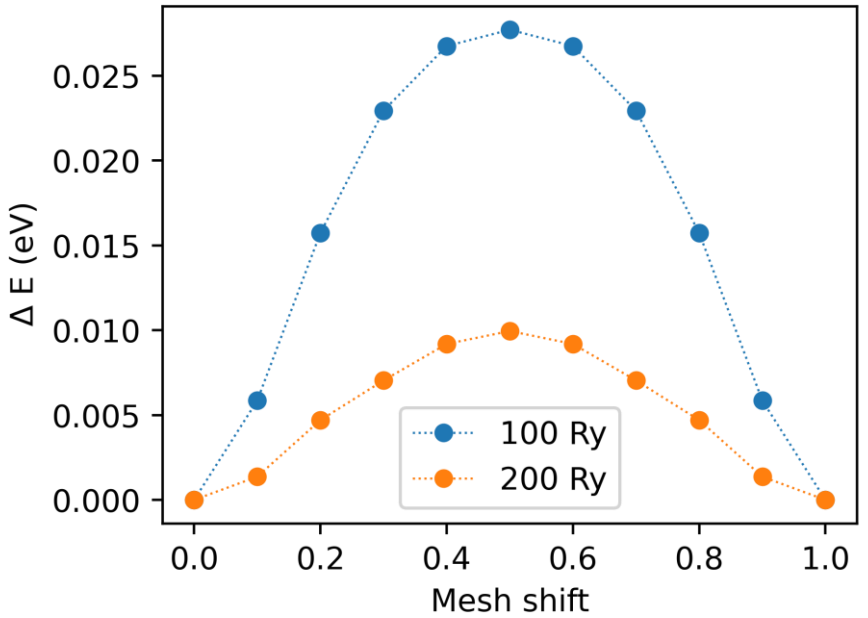


Results for methane (CH4)

Egg-box effect



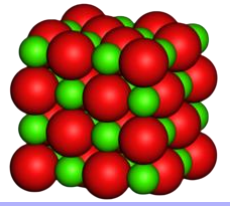
Invariant under any translation?




```
%block AtomicCoordinatesOrigin
 0.0 0.0 0.0
%endblock AtomicCoordinatesOrigin
```

Solution:
- Increase Meshcutoff
- Use “grid-cell-sampling”

$$\delta z_{shift} = \left(\frac{1}{M_z}\right)\frac{1}{10}$$



Results for magnesium oxide (MgO)

Let's try it

Tutorials

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day2/03-RealSpaceGrid

Reciprocal space grid

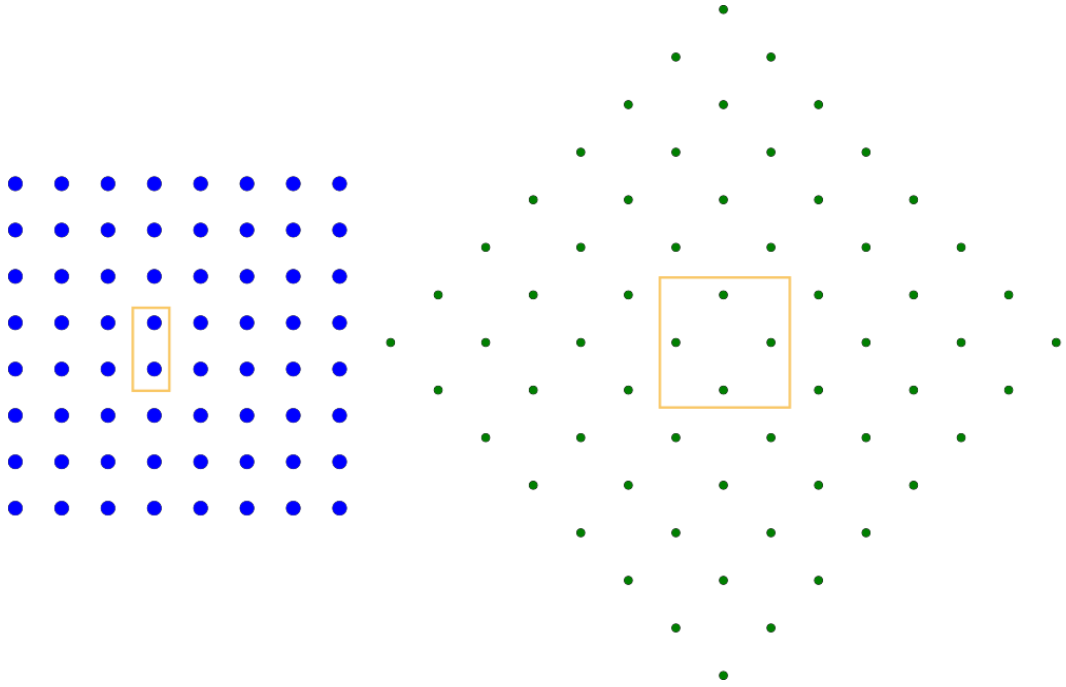
Crystals

$\psi(\mathbf{r})$
Infinite matrix

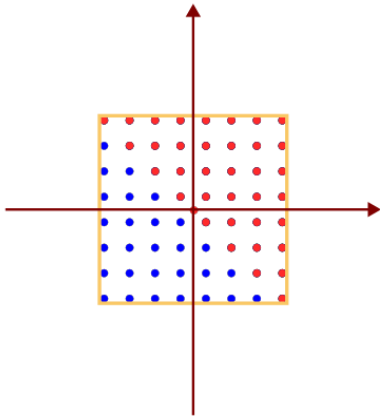
Periodicity

Reciprocal space
$\psi_{n,\mathbf{k}+\mathbf{G}}(\mathbf{r}) = \psi_{n,\mathbf{k}}(\mathbf{r})$

Finite matrix



$\psi_{up}(\mathbf{k}) = \psi_{down}(\mathbf{k})$



First Brillouin Zone

Reciprocal space grid: k-mesh

- What is it set by the user?
  - k grid cut off
  - Monkhorst Pack grid
- What is set by siesta?
  - SystemLabel.KP
- How can one decide the good value?
  - Must consider the ratio between the lattice vectors.
  - Check:
    - DOS
    - Bandstructure
  - For metallic systems more k points will be needed.

Input structure → Lattice vectors

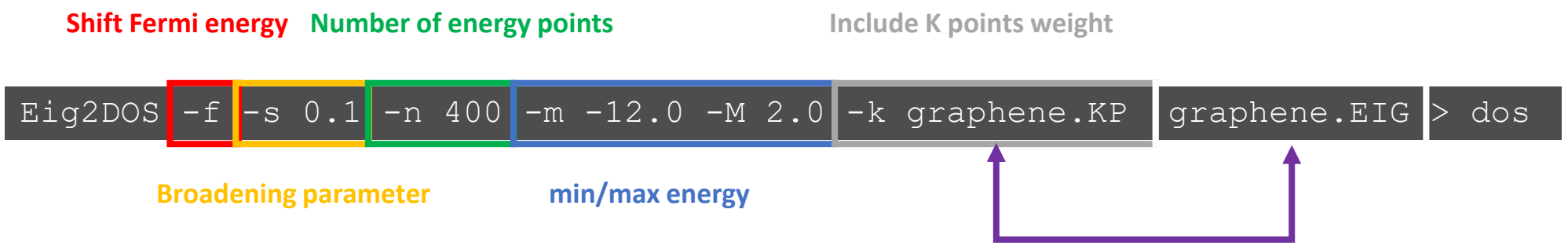
```
kgrid_cutoff          10.0 Ang
```

```
%block kgrid_Monkhorst_Pack
  6   0   0    0.0
  0   6   0    0.0
  0   0   1    0.0
%endblock kgrid_Monkhorst_Pack
```

SystemLabel.KP

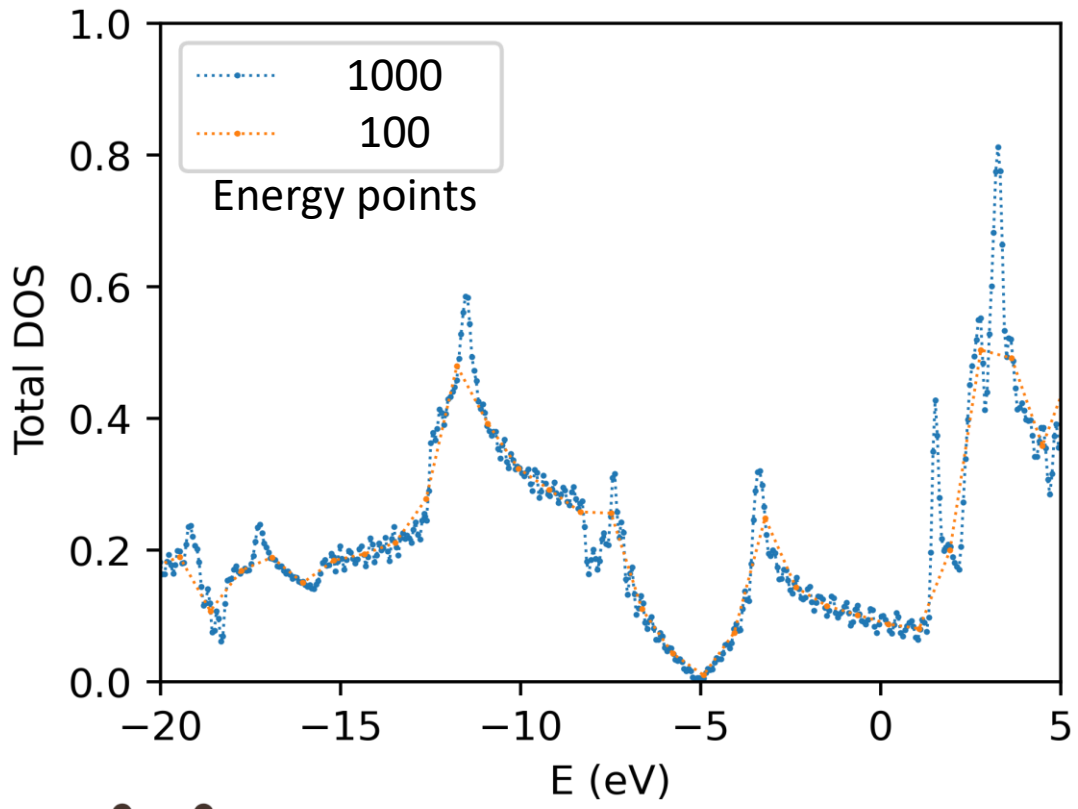
```
 22
 1 -0.447497E+00 -0.258363E+00  0.000000E+00   0.555556E-01
 2 -0.223749E+00 -0.129181E+00  0.000000E+00   0.555556E-01
 3  0.000000E+00  0.000000E+00  0.000000E+00   0.277778E-01
 4  0.671246E+00  0.387544E+00  0.000000E+00   0.277778E-01
 5 -0.447497E+00  0.111022E-15  0.000000E+00   0.555556E-01
 6 -0.223749E+00  0.129181E+00  0.000000E+00   0.555556E-01
 7  0.000000E+00  0.258363E+00  0.000000E+00   0.555556E-01
 8  0.223749E+00  0.387544E+00  0.000000E+00   0.555556E-01
 9  0.447497E+00  0.516726E+00  0.000000E+00   0.555556E-01
10  0.671246E+00  0.645907E+00  0.000000E+00   0.555556E-01
11 -0.447497E+00  0.258363E+00  0.000000E+00   0.555556E-01
12 -0.223749E+00  0.387544E+00  0.000000E+00   0.555556E-01
13  0.000000E+00  0.516726E+00  0.000000E+00   0.555556E-01
14  0.223749E+00  0.645907E+00  0.000000E+00   0.555556E-01
15  0.447497E+00  0.775088E+00  0.000000E+00   0.555556E-01
16  0.671246E+00  0.904270E+00  0.000000E+00   0.555556E-01
17 -0.447497E+00  0.516726E+00  0.000000E+00   0.277778E-01
18 -0.223749E+00  0.645907E+00  0.000000E+00   0.277778E-01
19  0.000000E+00  0.775088E+00  0.000000E+00   0.277778E-01
20  0.223749E+00  0.904270E+00  0.000000E+00   0.277778E-01
21  0.447497E+00  0.103345E+01  0.000000E+00   0.277778E-01
22  0.671246E+00  0.116263E+01  0.000000E+00   0.277778E-01
```

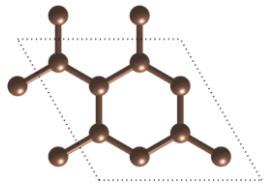
DOS: Eig2DOS


Shift Fermi energy
Number of energy points
Include K points weight
Eig2DOS -f -s 0.1 -n 400 -m -12.0 -M 2.0 -k graphene.KP graphene.EIG > dos
Broadening parameter
min/max energy

Eig2DOS output

```
 EIG2DOS: Utility for SIESTA to obtain the electronic density of states
#  E. Artacho, Apr 1999, A. Garcia, Apr 2012
#  Nick R. Papior, Feb 2017
# ----------------------------------------
# Eigenvalues calculated from a spin-polarized calculation
# Eigenvalues read from graphene.EIG
# Kpoint weights read from graphene.KP
# Using smearing parameter:   0.1000
# Using 400 points in the energy range
# Selected bands: 1 to: 26
# Emin, Emax in file for selected band(s):    -24.2236335    143.6658020
# Nbands, Nspin, Nk   =     26     2     5
# E_F                 =    -5.0301 eV --> (shifted to ZERO)
# Broadening          =     0.1000 eV
#
#        E            N(up)         N(down)         Ntot
    -12.000000      0.000000      0.000000      0.000000
    -11.964912      0.000000      0.000000      0.000000
    -11.929825      0.000000      0.000000      0.000000
    -11.894737      0.000000      0.000000      0.000000
    -11.859649      0.000000      0.000000      0.000000
    -11.824561      0.000000      0.000000      0.000000
    -11.789474      0.000000      0.000000      0.000000
    -11.754386      0.000000      0.000000      0.000000
    -11.719298      0.000000      0.000000      0.000000
    -11.684211      0.000000      0.000000      0.000000
    -11.649123      0.000000      0.000000      0.000000
    -11.614035      0.000000      0.000000      0.000000
    -11.578947      0.000000      0.000000      0.000000
    -11.543860      0.000000      0.000000      0.000000
    -11.508772      0.000000      0.000000      0.000000
    -11.473684      0.000000      0.000000      0.000000
    -11.438596      0.000000      0.000000      0.000000
    -11.403509      0.000000      0.000000      0.000000
    -11.368421      0.000000      0.000000      0.000000
    -11.333333      0.000000      0.000000      0.000000
    -11.298246      0.000000      0.000000      0.000000
    -11.263158      0.000000      0.000000      0.000000
    -11.228070      0.000000      0.000000      0.000000
    -11.192982      0.000000      0.000000      0.000000
    -11.157895      0.000000      0.000000      0.000000
    -11.122807      0.000000      0.000000      0.000000
    -11.087719      0.000000      0.000000      0.000000
    -11.052632      0.000000      0.000000      0.000000
    -11.017544      0.000000      0.000000      0.000000
    -10.982456      0.000000      0.000000      0.000000
    -10.947368      0.000000      0.000000      0.000000
    -10.912281      0.000000      0.000000      0.000001
```





Results for graphene

Bandstructure: gnubands

```
%block Bandlines
1    0.5000000000   0.000000000   0.0000   M
30    0.0000000000   0.000000000   0.0000   \Gamma
45    0.3333333333   0.333333333   0.0000   K
30    0.5000000000   0.500000000   0.0000   M
%endblock BandLines
```

SystemLabel.bands

-G : print GNUplot commands for correct labels to stderr
Suggested usage: prog options 2> bands.gplot 1> bands.dat
gnubands [options] 1> bands.dat 2> bands.gplot
and then:
gnuplot -persist bands.gplot
-s arg : only plot selected spin bands [1,nspin]
-F : shift energy to Fermi-level
-b arg : first band to write
-B arg : last band to write
-e arg : minimum energy to write
: If -F set, will be with respect
: to Fermi level
-E arg : maximum energy to write
: Note, see -e
-o file : specify output file (instead of piping)
: if used with -G a file name file.gplot will be created

Shift Fermi energy

```
gnubands -F -G -o bandstructure -E 10 -e -20 SystemLabel.bands
```

Shift Fermi energy

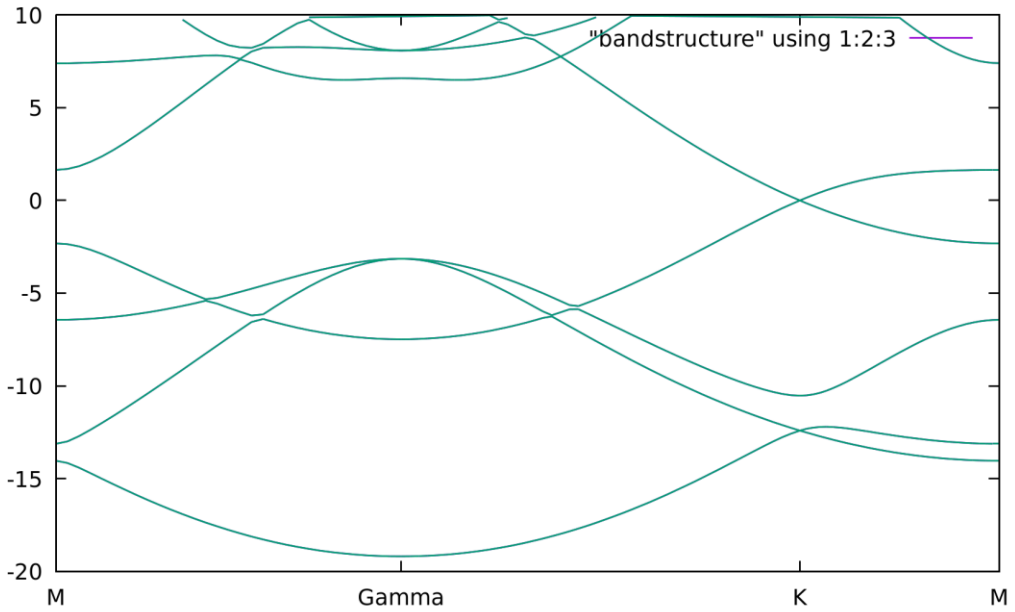
Min/max energy

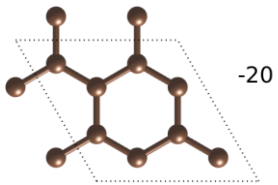
Bandstructure

```
gnubands -F -G -o bandstructure -E 10 -e -20 *.bands

gnuplot -persist bandstructure.gplot
```

```
set xtics ("M"  0.000000, "Gamma"  0.775088, "K"  1.670083, "M"  2.117581)
plot "bandstructure" using 1:2:3 with lines lc variable
# -- Use line below for single-color#plot "bandstructure" with lines
```





Results for graphene

```
# GNUBANDS: Utility for SIESTA to transform bands output into
#Gnuplot format
#
# Emilio Artacho, Feb. 1999 # Alberto Garcia, May 2012
# Nick Papior, April 2013, July 2016
# ---------------------------------------------------------------------
# Bands for all spins
# E_F / orig = 0.0000 -5.0301
# k_min, k_max = 0.0000 2.1176
# E_min, E_max = -20.0000 10.0000
# Nbands, Nspin, Nk = 26 2 106
# Using min_band, max_band = 1 26
# Total number of bands = 26
#
# k E[eV]
# ---------------------------------------------------------------------
0.000000 -14.038730 1
0.025836 -14.158130 1
0.051673 -14.413430 1
0.077509 -14.707530 1
0.103345 -15.009230 1
0.129181 -15.308430 1
0.155018 -15.601030 1
0.180854 -15.885030 1
0.206690 -16.159330 1
0.232526 -16.423330 1
0.258363 -16.676430 1
0.284199 -16.918530 1
0.310035 -17.149230 1
```

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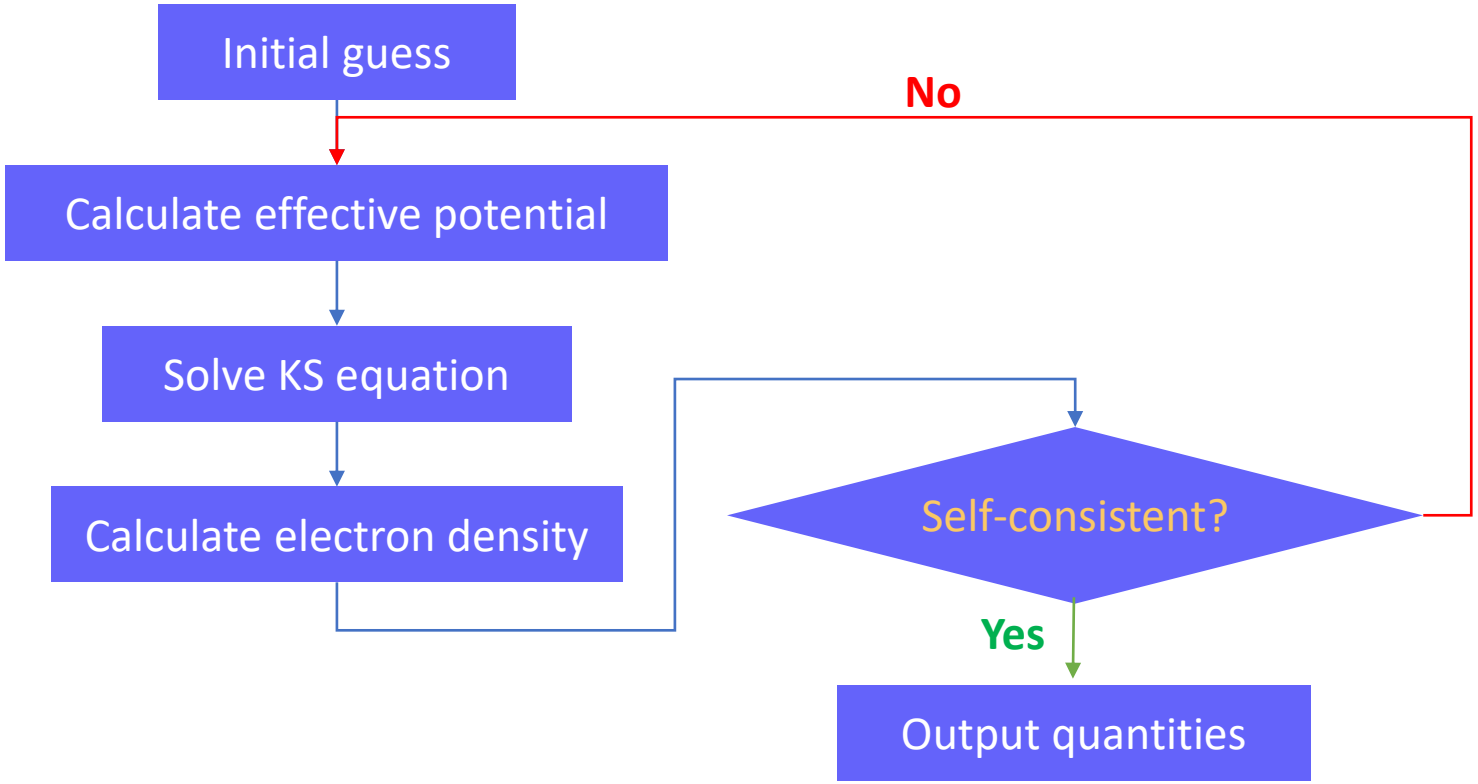
day2/04-KpointSampling

SCF convergence

SCF convergence



- The physical quantity that is mixed:
  - Density matrix
  - Hamiltonian matrix
- Mixing algorithm:
  - Linear
  - Broyden
  - Pulay

} N previous steps

SCF convergence

- SCF.Mix [default Hamiltonian]:
  - Density -> for systems hard to converge
  - Hamiltonian
- SCF.MixerMethod [default Pulay]
  - Linear
  - Pulay
  - Broyden
- SCF.Mixer.Weight [default 0.25]
  - 0.001 systems hard to converge ->a lot of steps
  - 0.4 systems easy to converge -> reduce steps
- SCF.Mixer.History [default 2]
- Max.SCF.Iterations [default 1000]
- SCF.DM.Converge F [default T]
- SCF.H.Converge F [default T]

All of them strongly dependent on the system!!

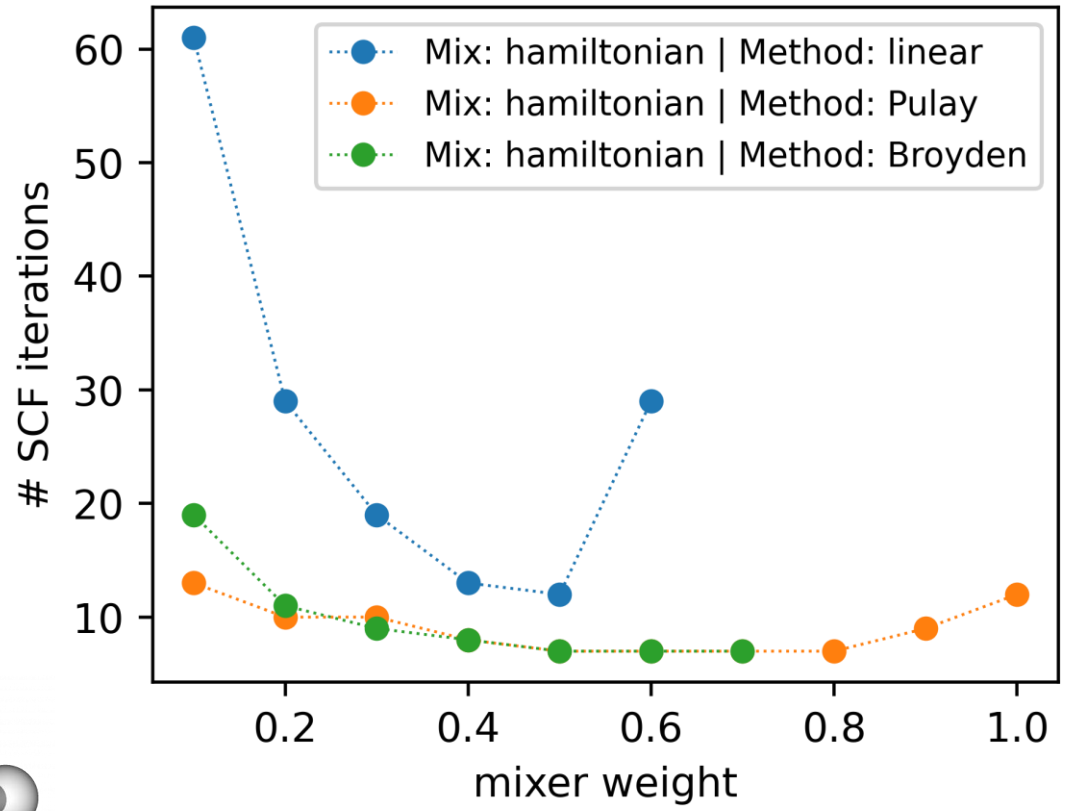
```
SCF.Mix Hamiltonian
SCF.MixerMethod Pulay
SCF.Mixer.Weight 0.3

SCF.DM.Tolerance 10-4
SCF.H.Tolerance 10-3 eV

Max.SCF.Iterations 75
SCF.MixerMethod pulay
SCF.Mixer.Weight 0.2

SCF.Mixer.History 5
```

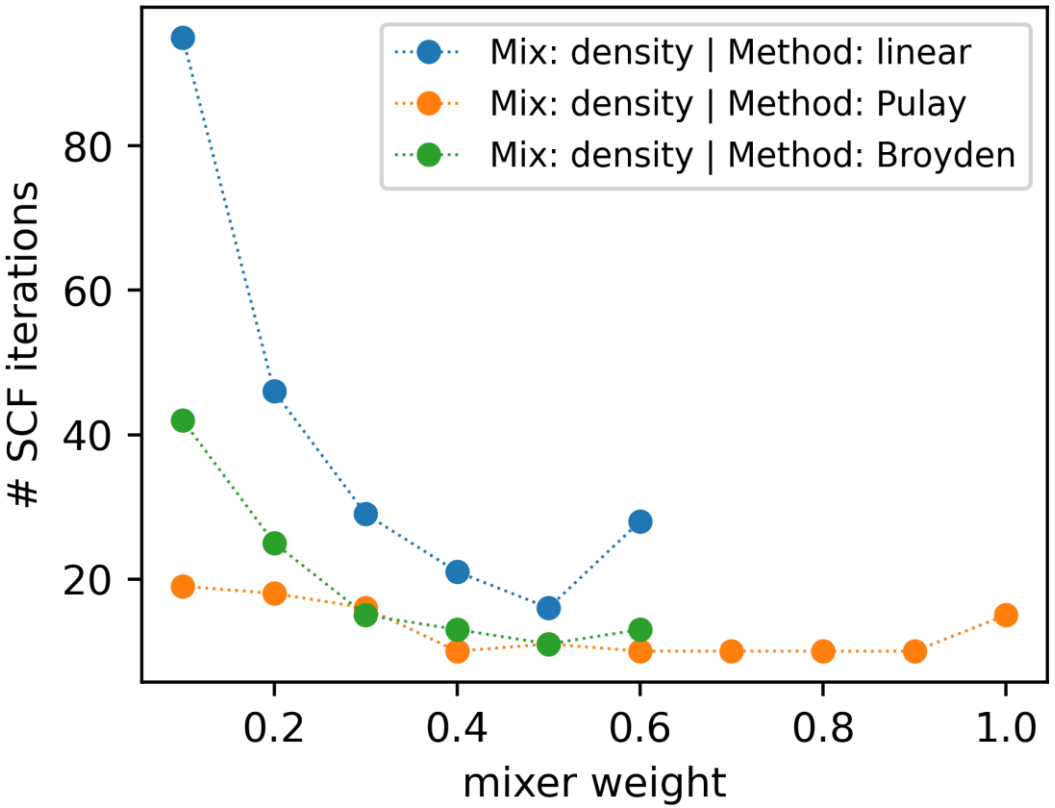
More advanced options … (manual)

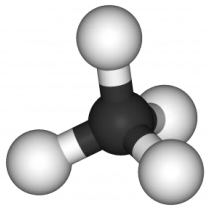
SCF convergence

```
SCF cycle converged
```

```
SCF_NOT_CONV:
```







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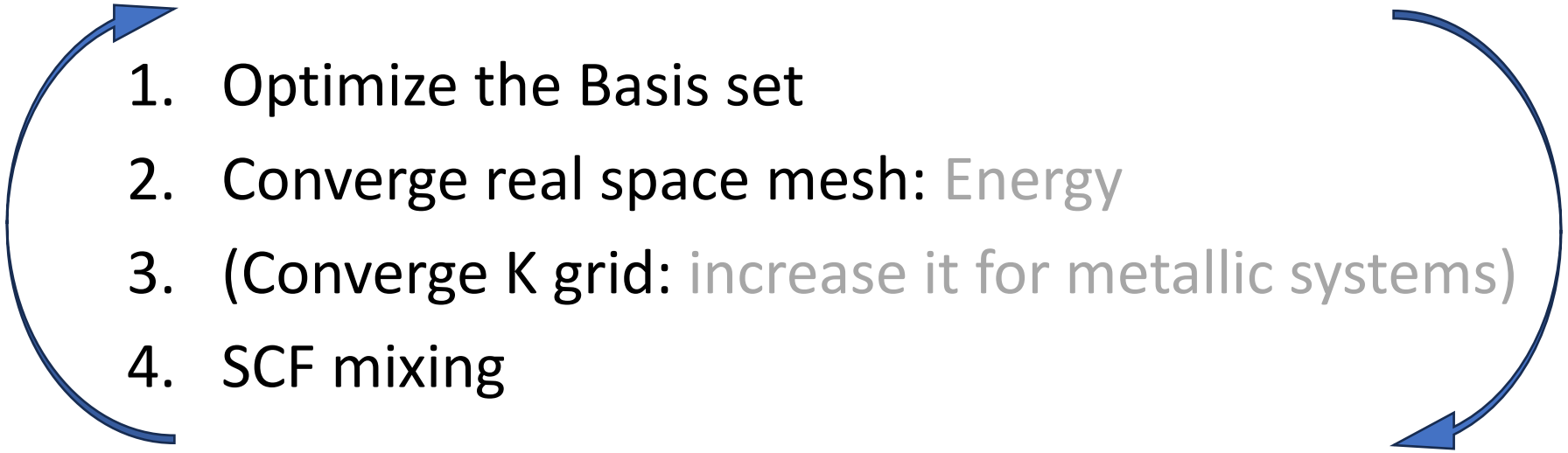
day2/05-SCF-Options

How do I converge the whole calculation?



1. Optimize the Basis set
2. Converge real space mesh: Energy
3. (Converge K grid: increase it for metallic systems)
4. SCF mixing

siesta
TM

Thank you for your attention

MAX DRIVING THE EXASCALE TRANSITION

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Centre Européen de Calcul Atomique et Moléculaire

BSC Barcelona Supercomputing Center
Centro Nacional de Supercomputación

ICN2
Institut Català de Nanociència i Nanotecnologia