Converging siesta calculations

Mesh, k-points and SCF convergence: hands on

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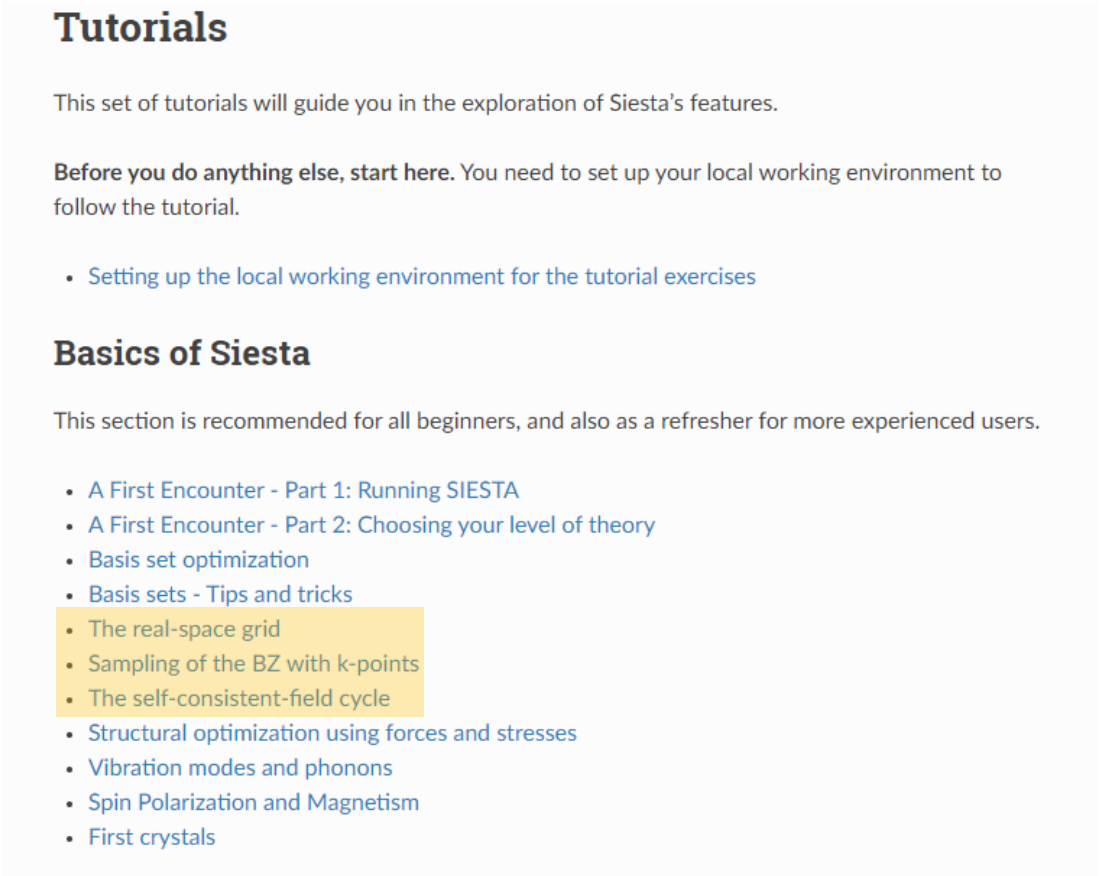
MAX DRIVING THE EXASCALE TRANSITION
ICN2 Institut Català de Nanociència i Nanotecnologia
EXCELENCIA SEVERO OCHOA 07/2014 - 06/2018 07/2018 - 06/2022 2023 - 2026
Funded by MINISTERIO DE CIENCIA E INNOVACIÓN
AGENCIA ESTATAL DE INVESTIGACIÓN

Quality/accuracy/precision

Time (CET)	Topic
09:00-09:45	SIESTA basics
09:45-10:30	A first contact with SIESTA: inputs, execution and outputs
10:30-10:45	Break
10:45-11:30	Basis sets
11:30-12.00	Basis set optimization
12:00-13:00	Convergence (K points, Mesh, Mixing)



Tutorials

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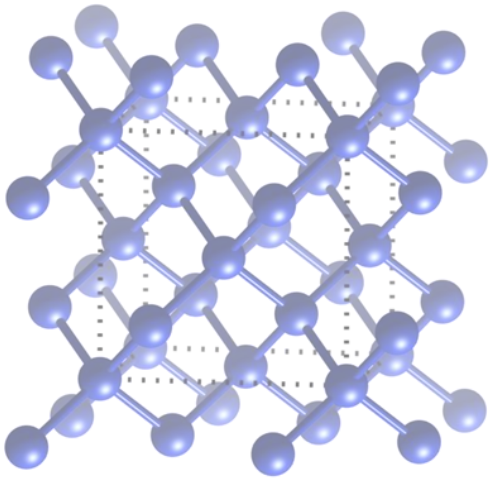
```
cp /leonardo_work/EUHPC_TD02_030/siesta-tutorials/day3-wed/04* ./
```

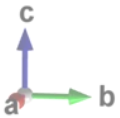
Sampling

Sampling

Real space

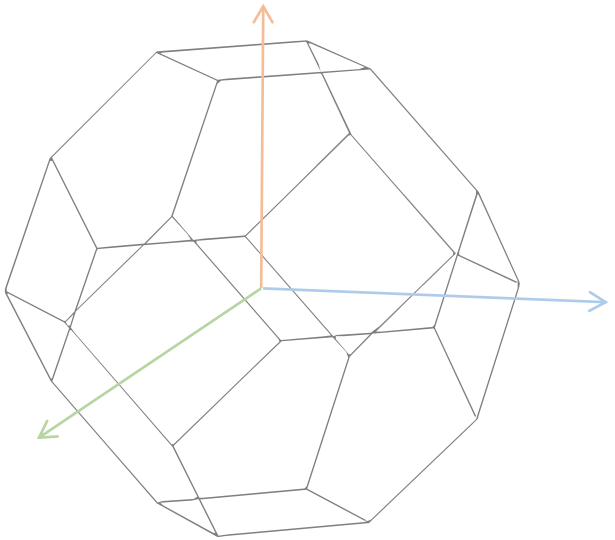
- **Potentials**
- **Densities**
- **Basis**



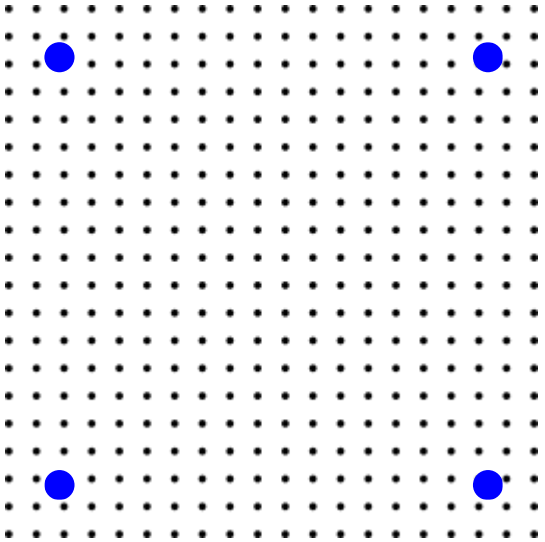


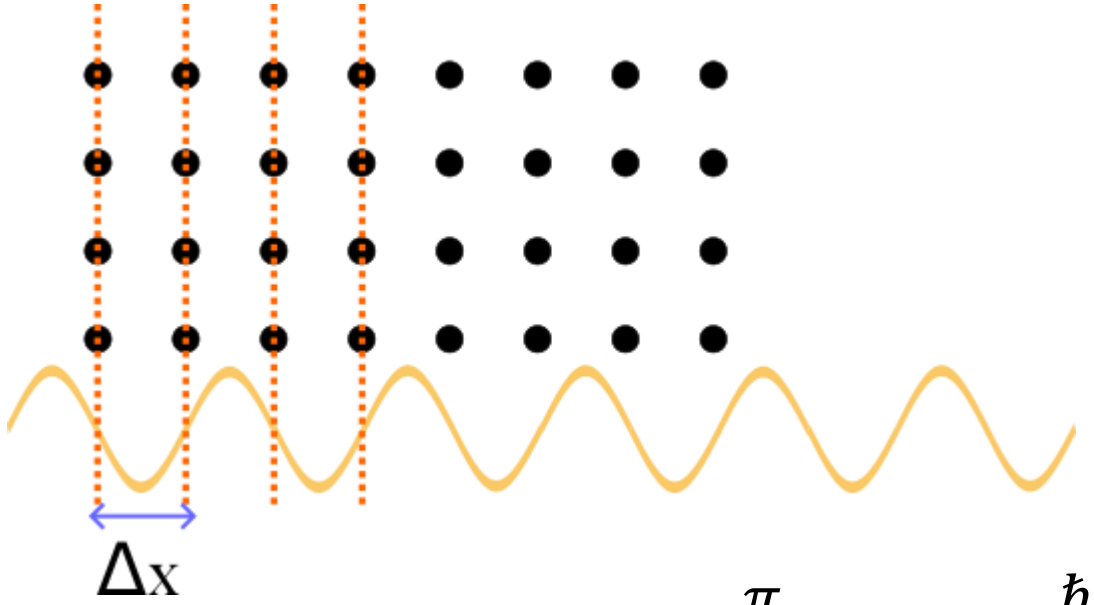
Reciprocal space

- **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)

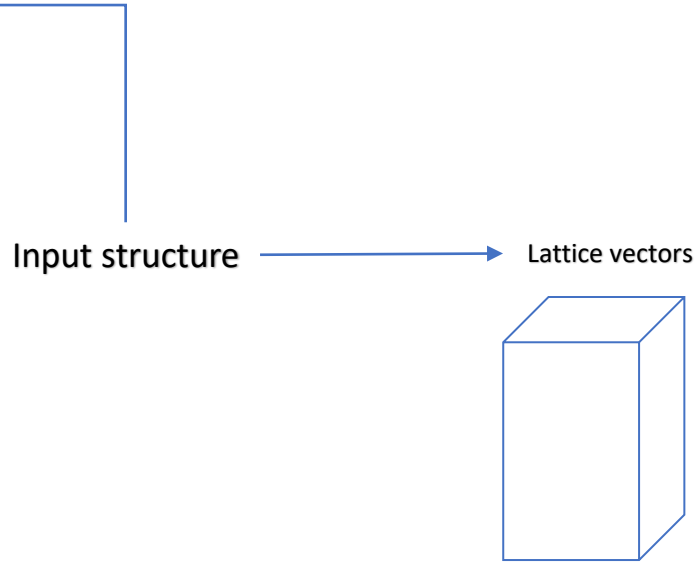
Real space grid: MeshCutoff

- 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

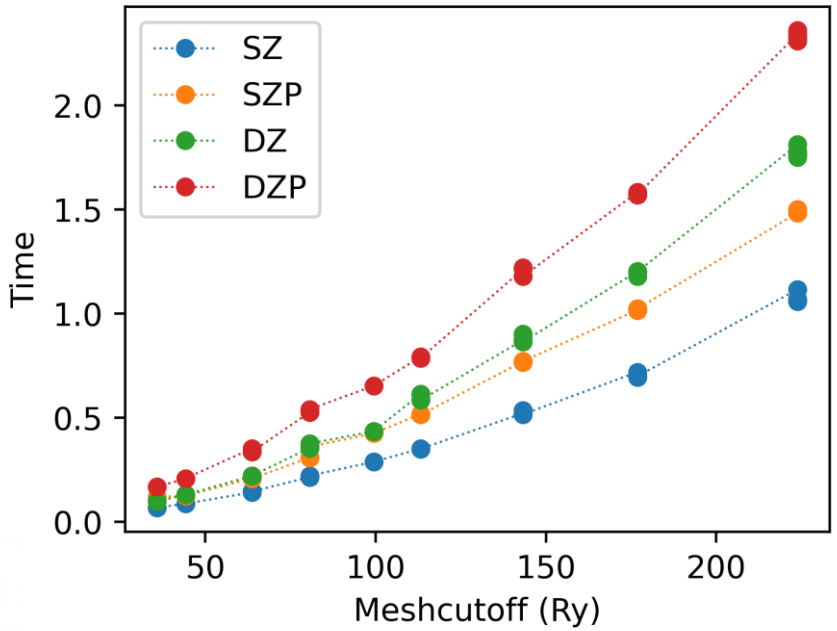
- How can one decide the good value?
  - Minimize the total energy.
  - Total force to zero.
  - Reasonable time (relatively small systems)



Real space grid: MeshCutoff

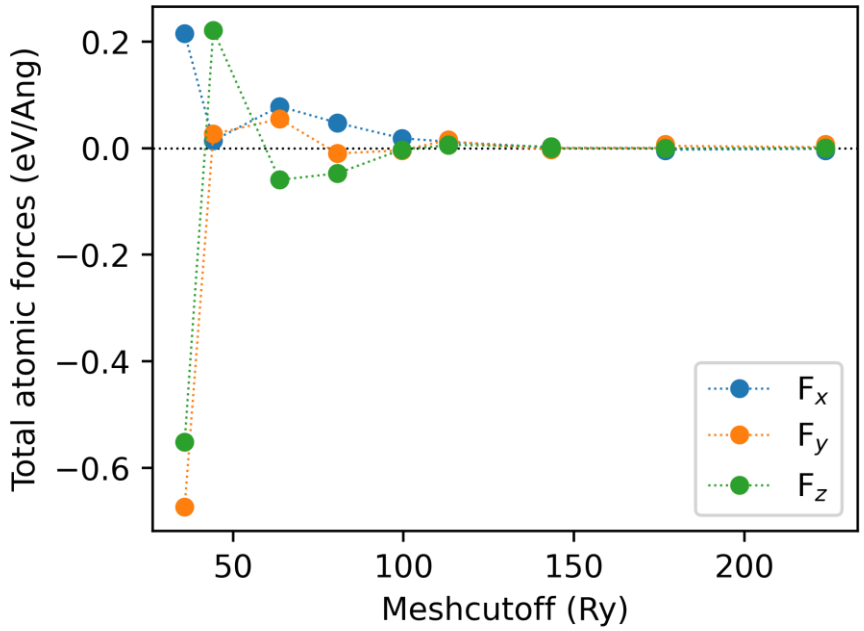
Time

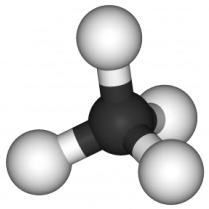
`TIMES file`



Force

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



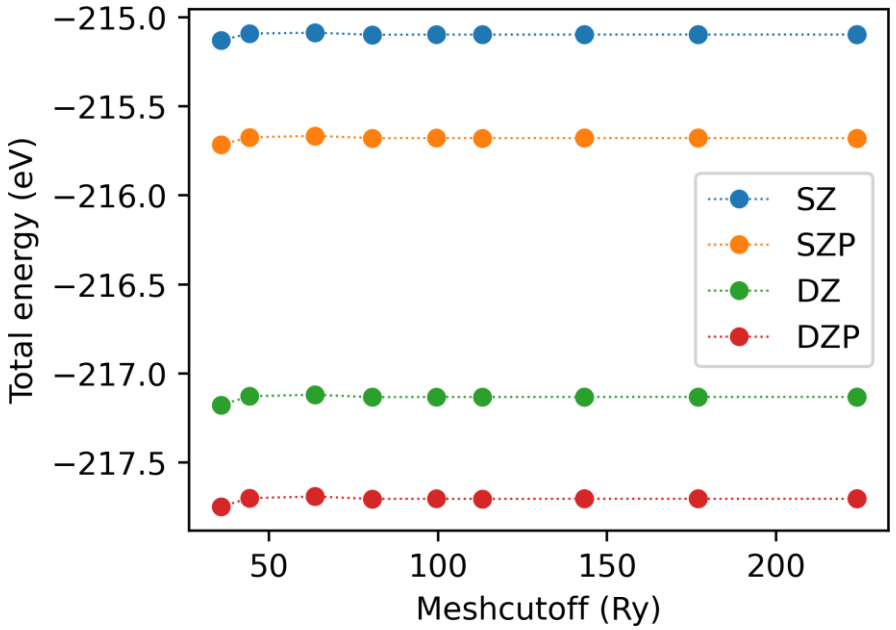


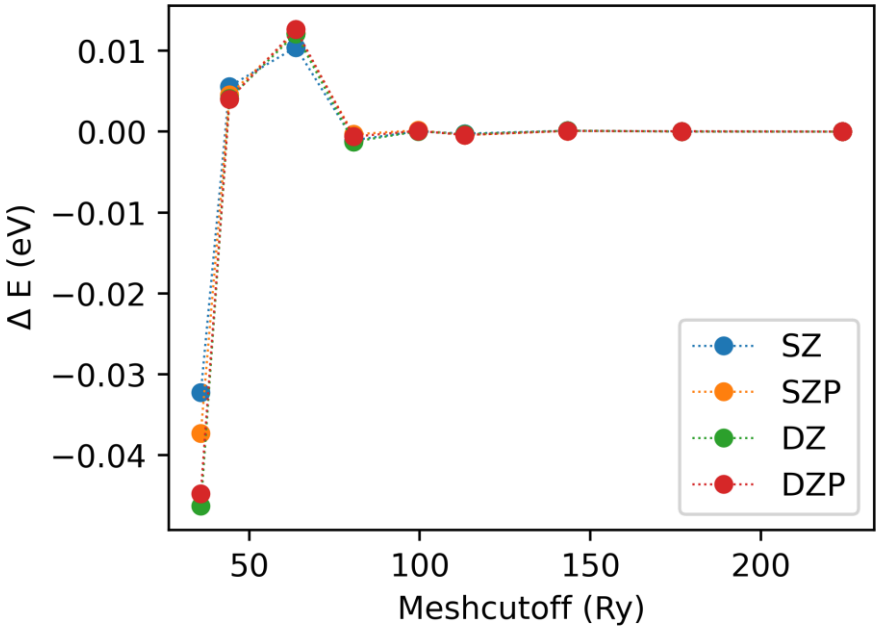
Results for methane (CH4)

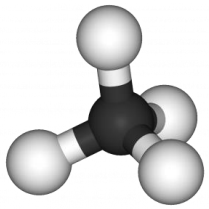
Real space grid: MeshCutoff

Energy

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







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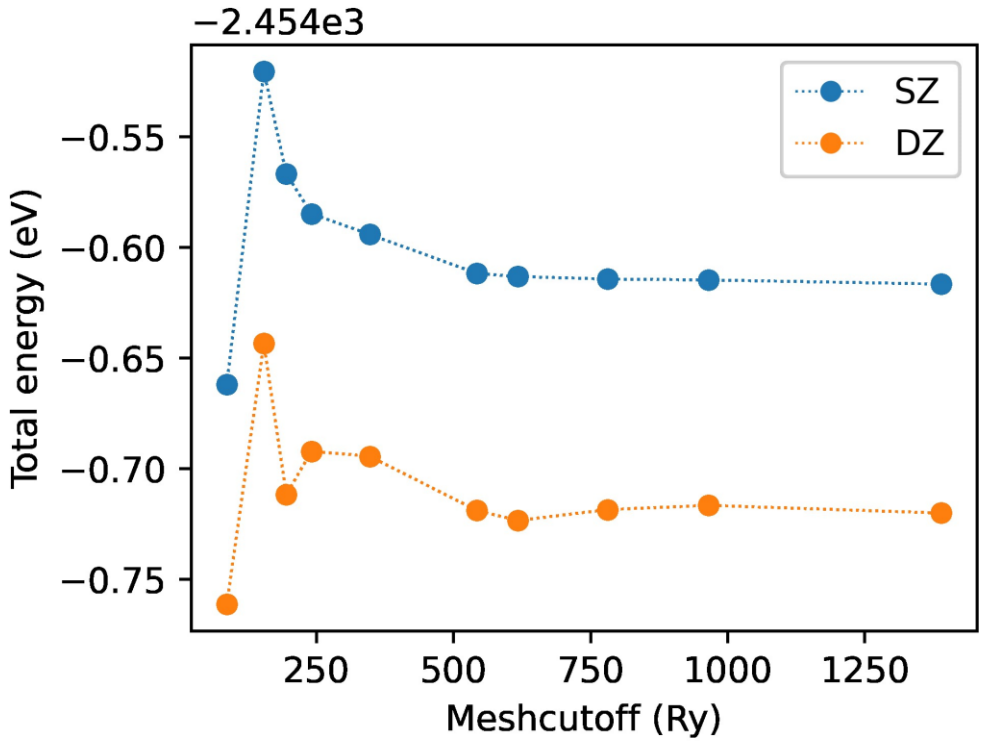
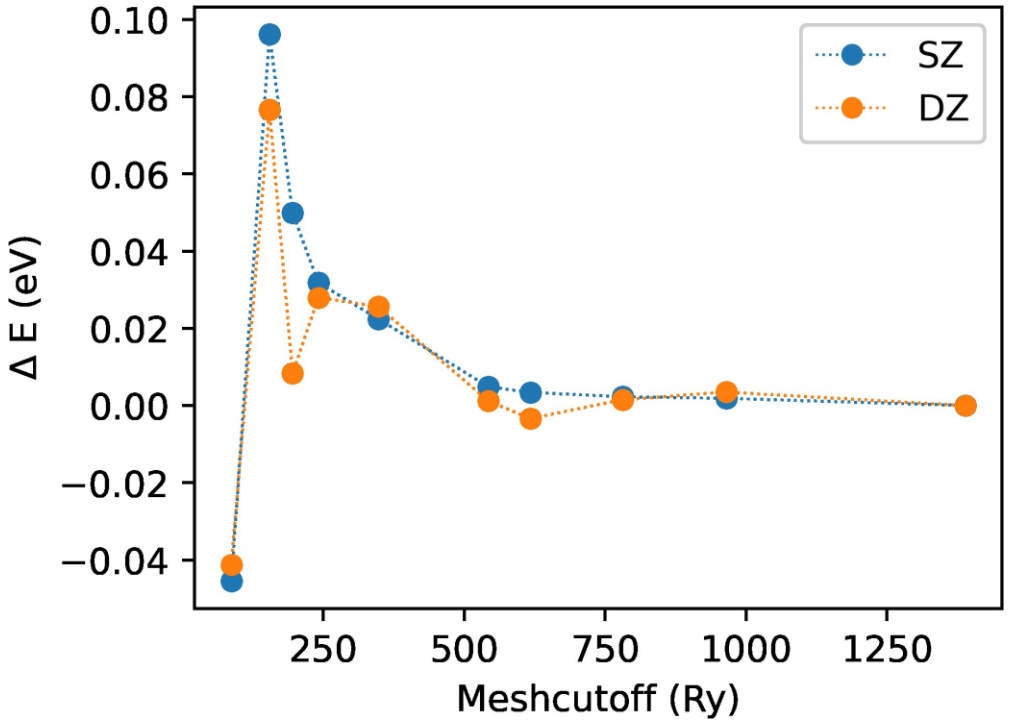
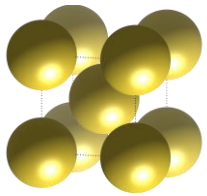
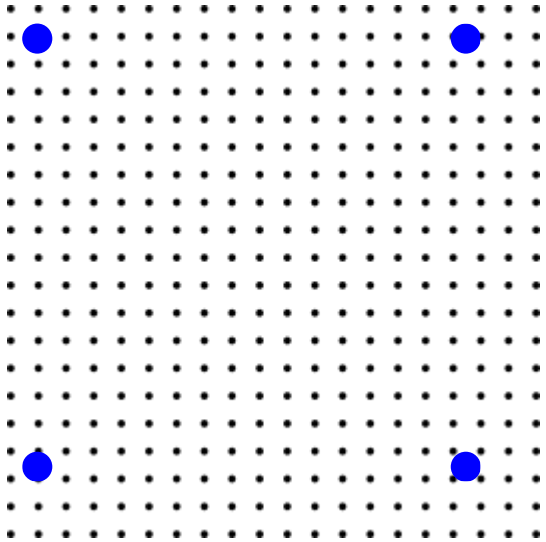




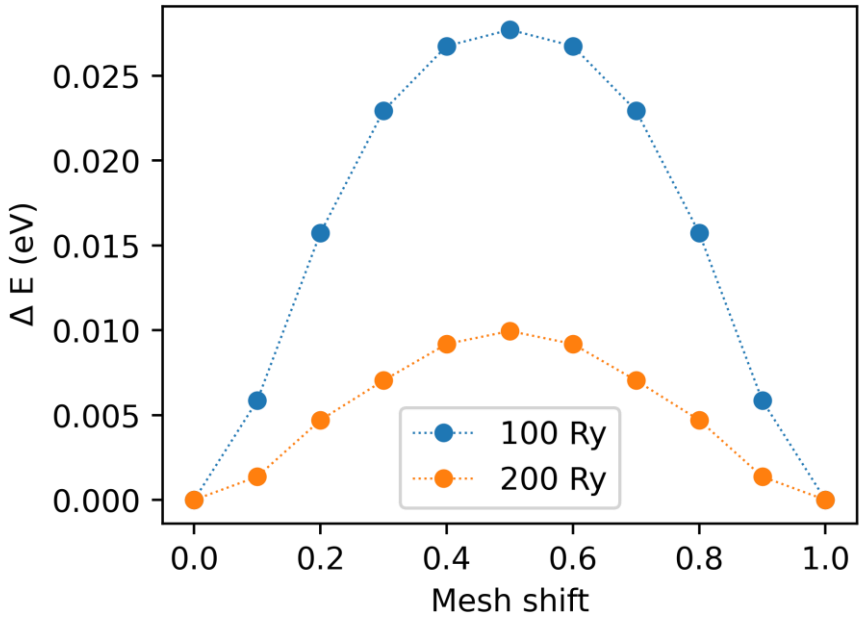


Results for sodium (Na)

Egg-box effect



Invariant under any translation?

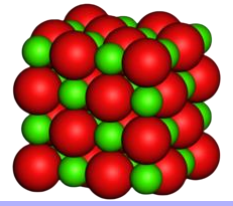



```
%block AtomicCoordinatesOrigin
 0.0 0.0 0.0
%endblock AtomicCoordinatesOrigin
```

Solutions:

- 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

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Day3-wed/04a-GridConvergence

Reciprocal space grid

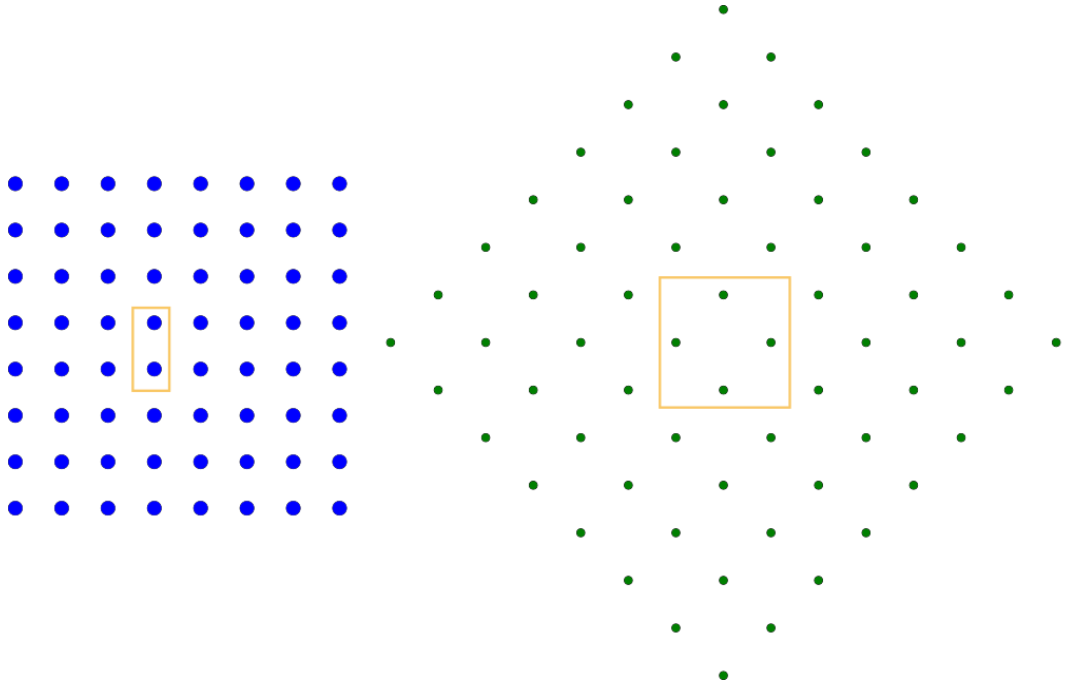
Crystals

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

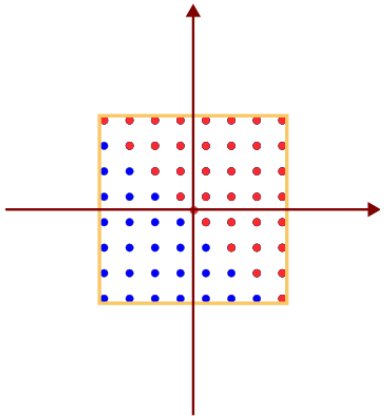
Periodicity

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: Energy
    - DOS
    - Bandstructure
  - For metallic systems more k points will be needed.

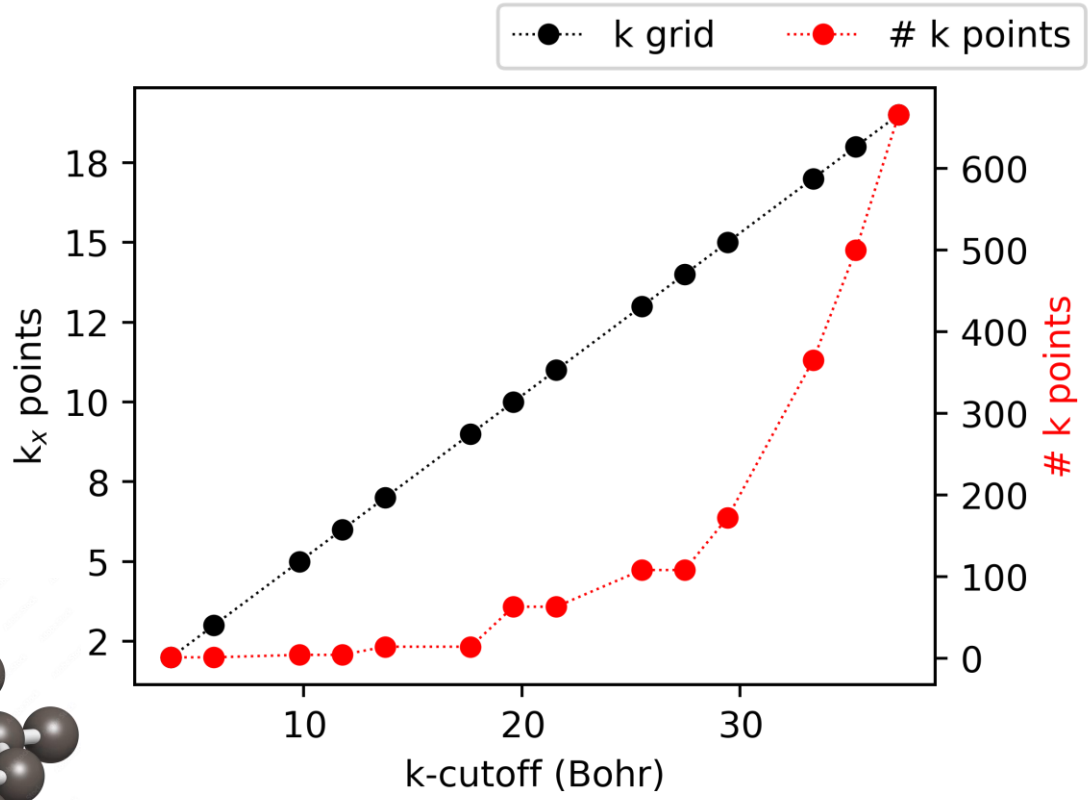
Input structure → Lattice vectors

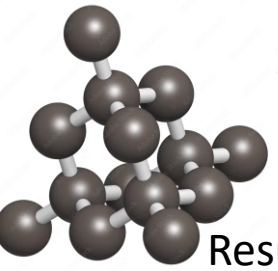
```
kgrid_cutoff          10.0 Ang

%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

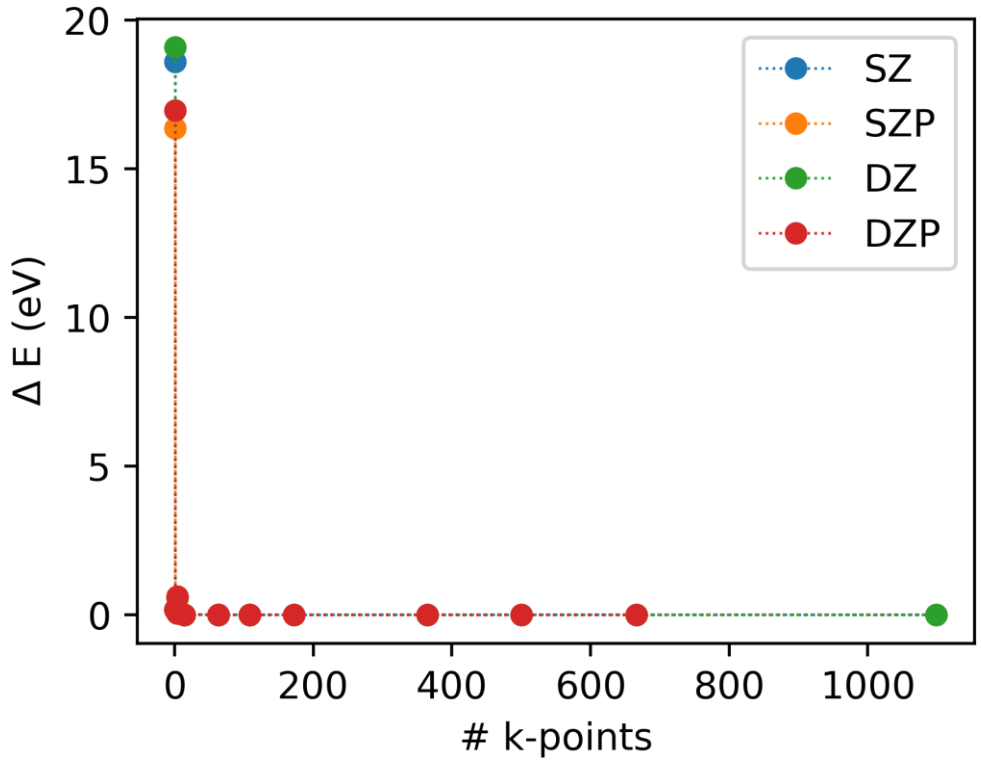
	Coordinates (Bohr^{-1})			Weight
22				
1	-0.447497E+00	-0.258363E+00	0.000000E+00	0.555556E-01
2	-0.223749E+00	-0.129181E+00	0.000000E+00	0.555556E-01
3	0.000000E+00	0.000000E+00	0.000000E+00	0.277778E-01
4	0.671246E+00	0.387544E+00	0.000000E+00	0.277778E-01
5	-0.447497E+00	0.111022E-15	0.000000E+00	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

k sampling



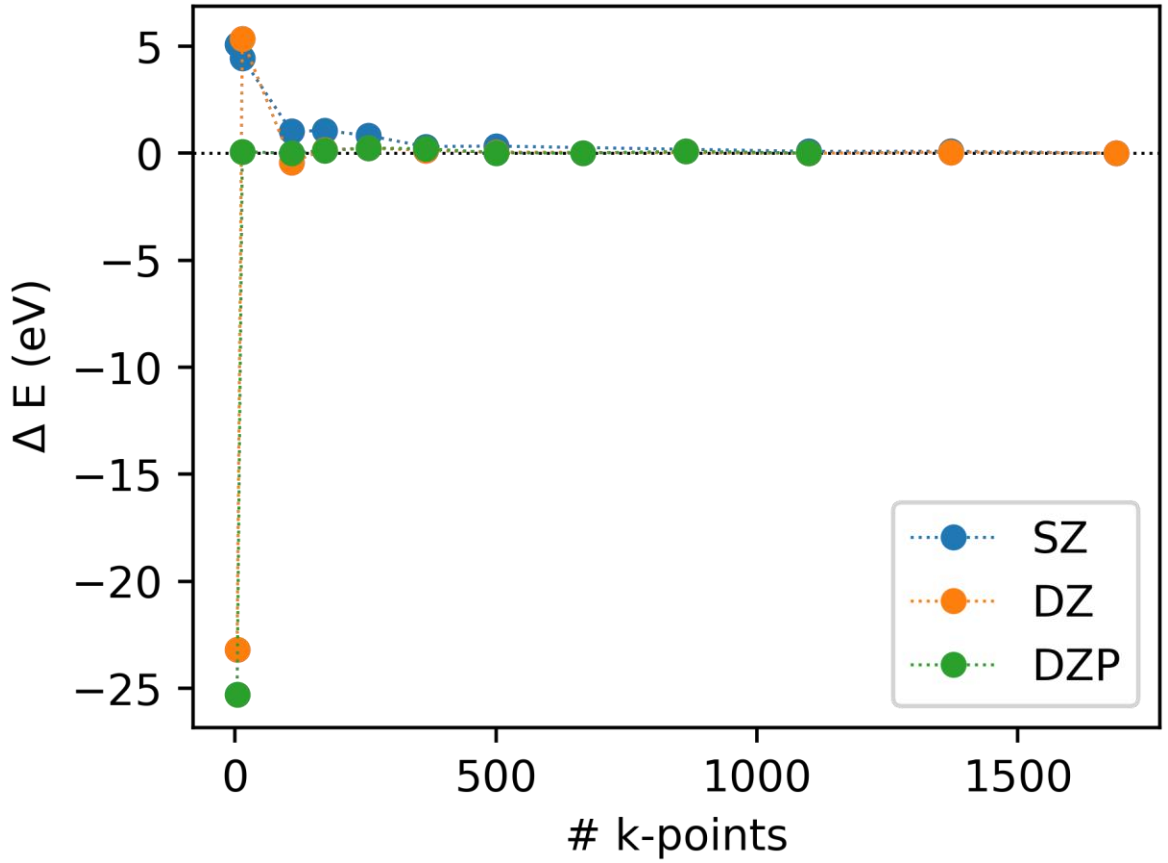


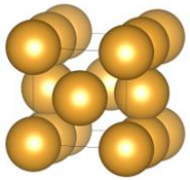
Results for silicon (Si)




```
Gamma-point calculation with interaction between
periodic images Some features might not work optimally
```

Metallic systems





Results for gold (Au)

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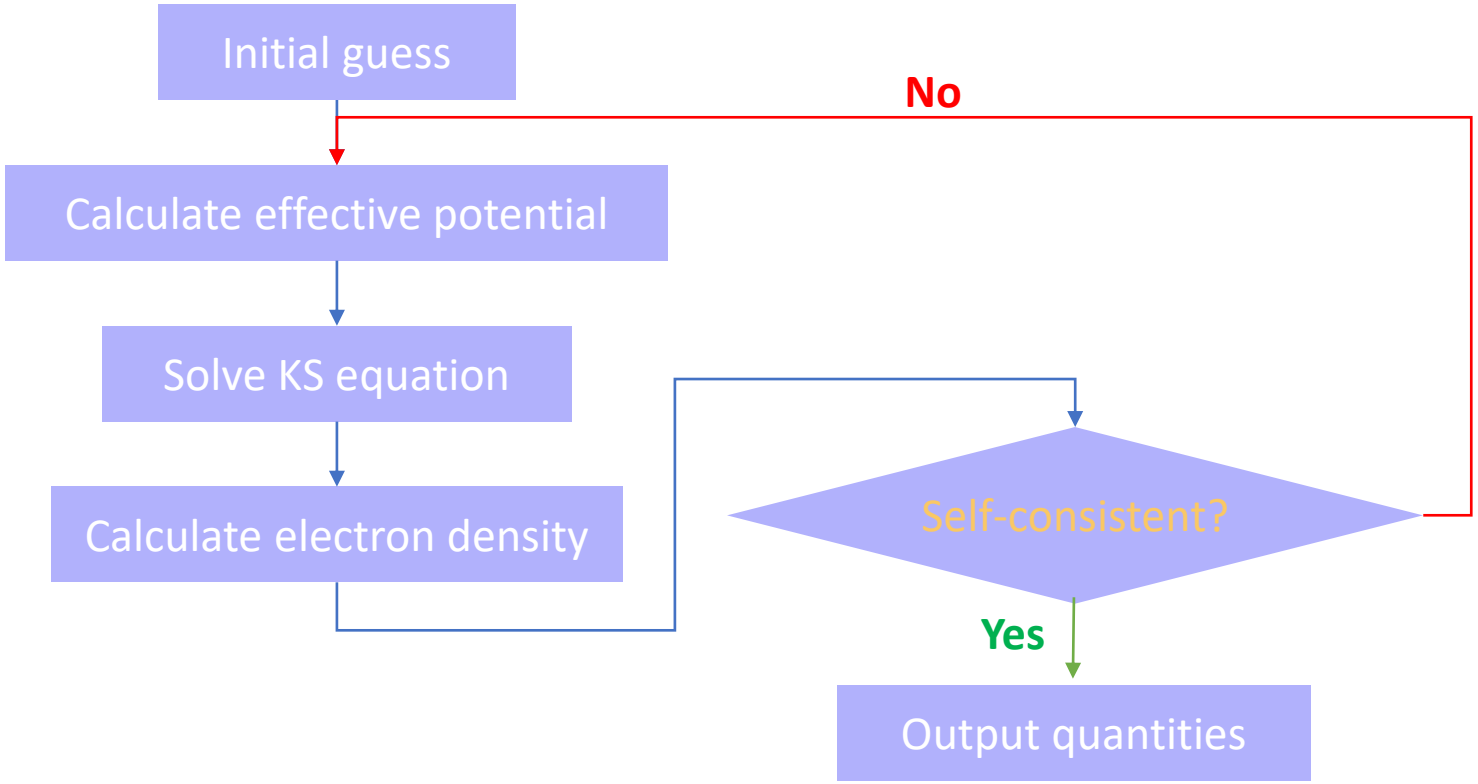
SCF convergence

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

Max.SCF.Iterations 75

SCF.MixerMethod pulay
SCF.Mixer.Weight 0.2

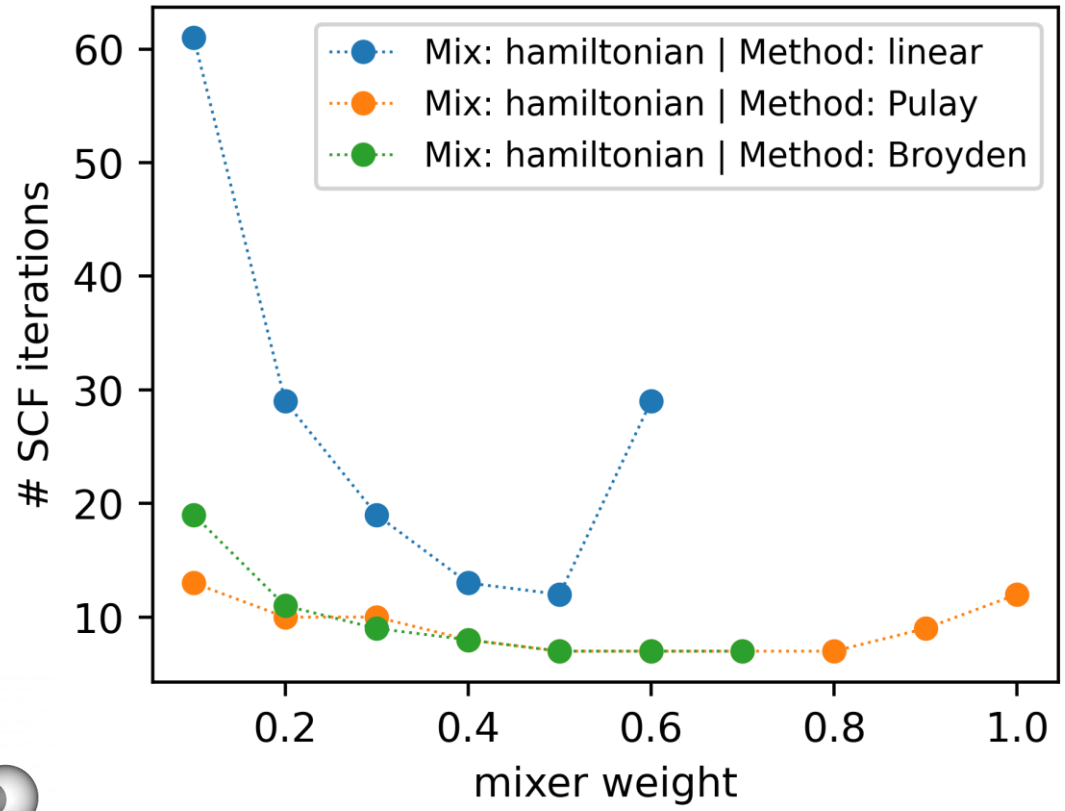
SCF.Mixer.History 5

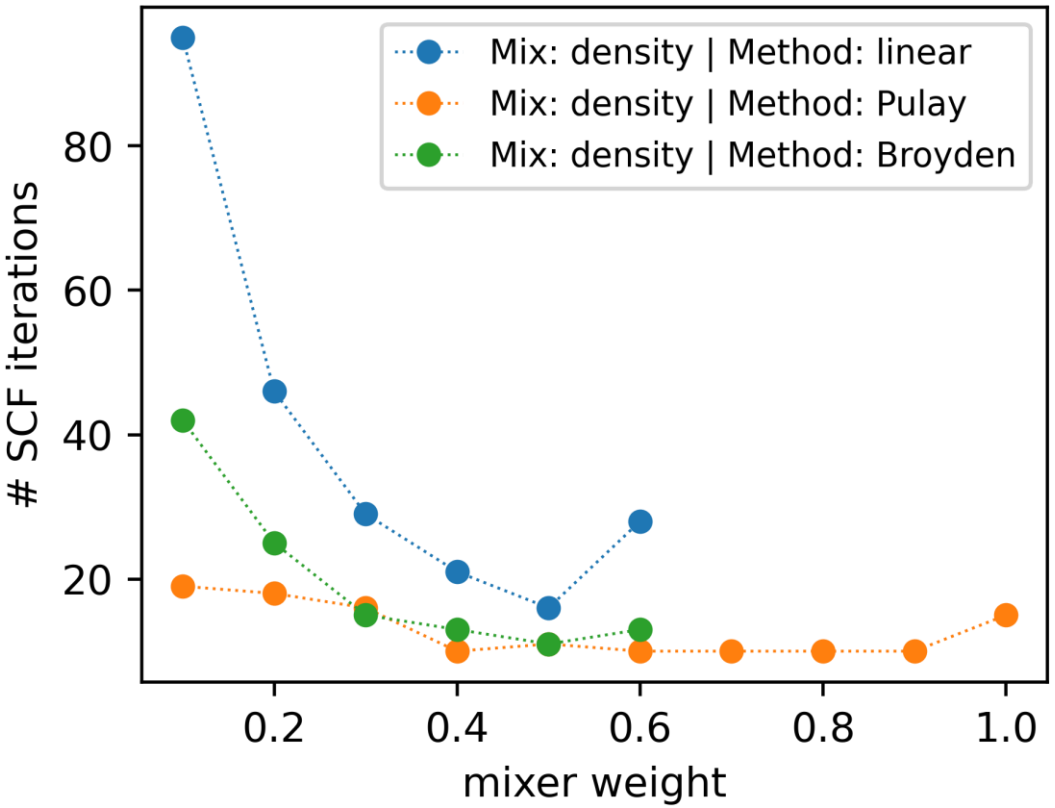
More advanced options … (manual)

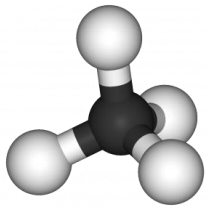
SCF convergence

```
SCF cycle converged
```

```
SCF_NOT_CONV:
```

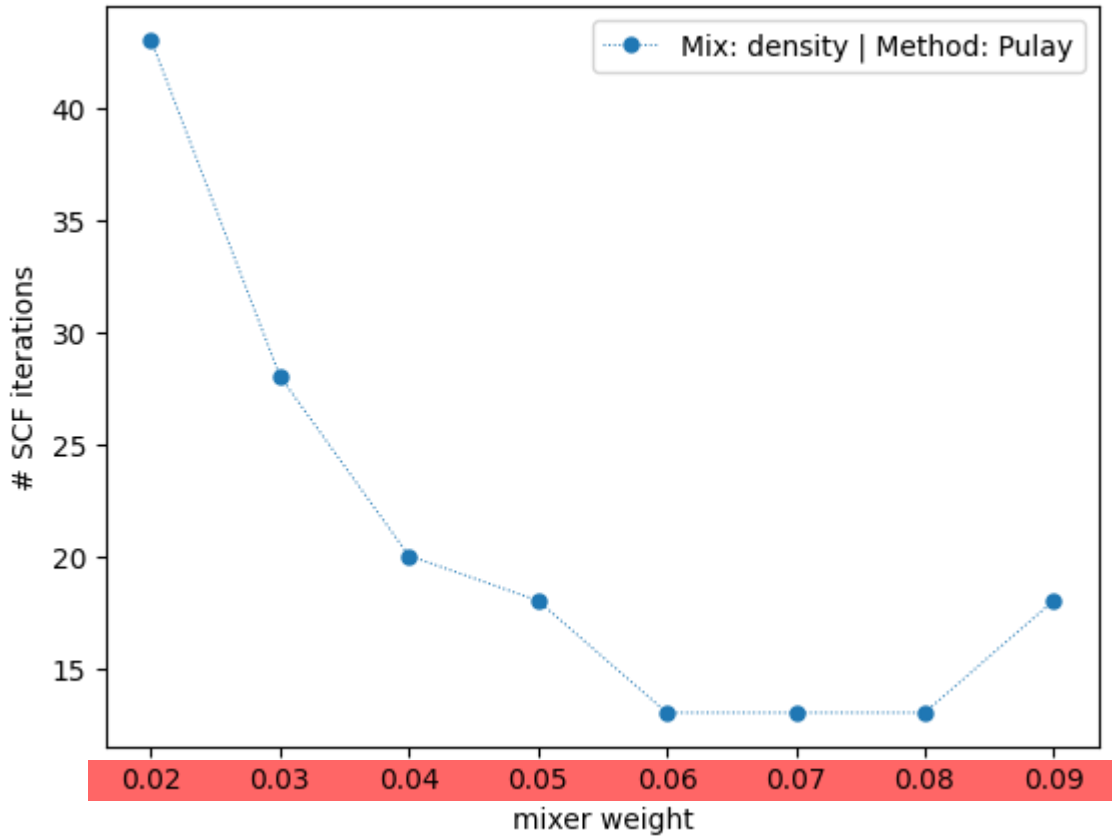


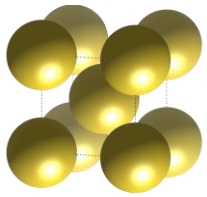




Results for methane (CH4)

Systems hard to converge





Results for sodium (Na)

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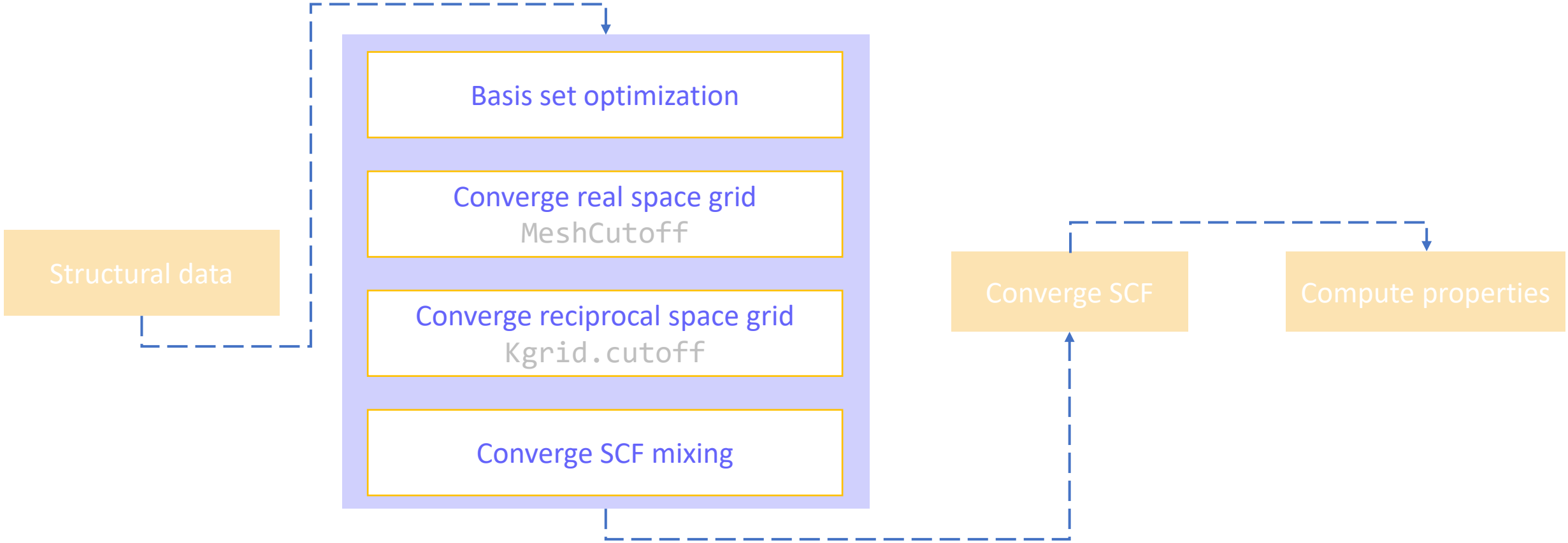
day3-wed/04c-SCF

How do I converge the whole calculation?



siesta
TM

Thank you for your attention

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SEVERO
OCHOA
07/2014 - 06/2018
07/2018 - 06/2022
2023 - 2026

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