A first contact with siesta

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MAX DRIVING THE EXASCALE TRANSITION

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AGENCIA ESTATAL DE INVESTIGACIÓN

ICN2 Institut Català de Nanociència i Nanotecnologia

Where to find the course materials?

https://siesta-project.org/siesta/index.html

siesta

siesta

What is SIESTA?

Getting the code

Documentation

Support

News

Events

The Team

For Developers

https://siesta-project.org/siesta/index.html

siesta

siesta

Home | What is SIESTA? | Getting the code | Documentation | Support | News | Events | The Team | For Developers

Events

Ongoing and future events

- Materials Science from First Principles: Materials Scientist Toolbox (3rd - 7th November 2025)
- SIESTA School 2025 (17th - 21th November 2025)

Past events

- Advanced SIESTA Workshop 2025 (2nd - 5th June 2025)
- SIESTA School 2024 (11th - 15th November 2024)
- The East-African School on Density Functional Theory and its Applications (8th - 10th July 2024)
- Efficient materials modelling on HPC with QUANTUM ESPRESSO, SIESTA and Yambo (11th - 15th March 2024)
- TranSIESTA School 2023 (13th - 17th November 2023)
- First steps with SIESTA: from zero to hero (2nd - 6th October 2023)
- First-principles simulations of materials with SIESTA (28th June - 2nd July 2021)
- Advanced school on Quantum Transport using SIESTA (17th May - 21st May 2021)
- Spin-orbit coupling in Siesta: Magnetism and other capabilities (20th June - 22nd June 2018)
- MaX SIESTA Tutorial 2017 (23rd May - 26th May 2017)

https://siesta-project.org/siesta/index.html

SIESTA School 2025

17th - 21th November 2025 (online)

Summary

The school is aimed at students and researchers from different disciplines who already use, or plan to use, first-principles techniques to simulate properties of matter at the atomic scale. In particular, the school will focus on the SIESTA method [1,2]. Participants will learn its essential theoretical foundations, and how to use the SIESTA code effectively. Pre- and post-processing tools will also be presented.

Format

The School will consist of lectures from senior SIESTA developers and hands-on sessions where SIESTA experts will be available for discussion and guidance. These sessions will take place between 12:30 CET and 17:30 CET.

Autonomous work on the exercises will be possible throughout the day.

You may find detailed information on the planned sessions and tutorials here.

Course materials

The school will make extensive use of the Siesta Project Documentation site, which is continuously updated with new tutorials.

The hands-on sessions will involve the execution of software, including pre-compiled versions of SIESTA, on users' computers. Indications on how to install the required software with conda will be provided to accepted participants well in advance.

Registration

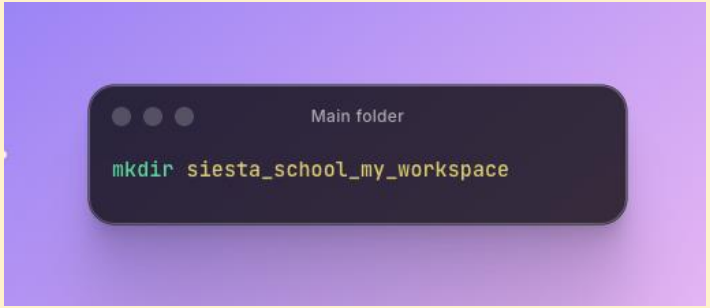
Persons interested in registering for the School need to apply through the "Participate" tab of the CECAM school web page.

Please make sure that your CECAM account is up to date and uses your current email address.

The deadline for applications is the **17th October 2025**.

Setup and organization of your workspace

- Create your main folder



/siesta_school_my_workspace/

This folder will contain all the folders and files for this school.

Siesta documentation site

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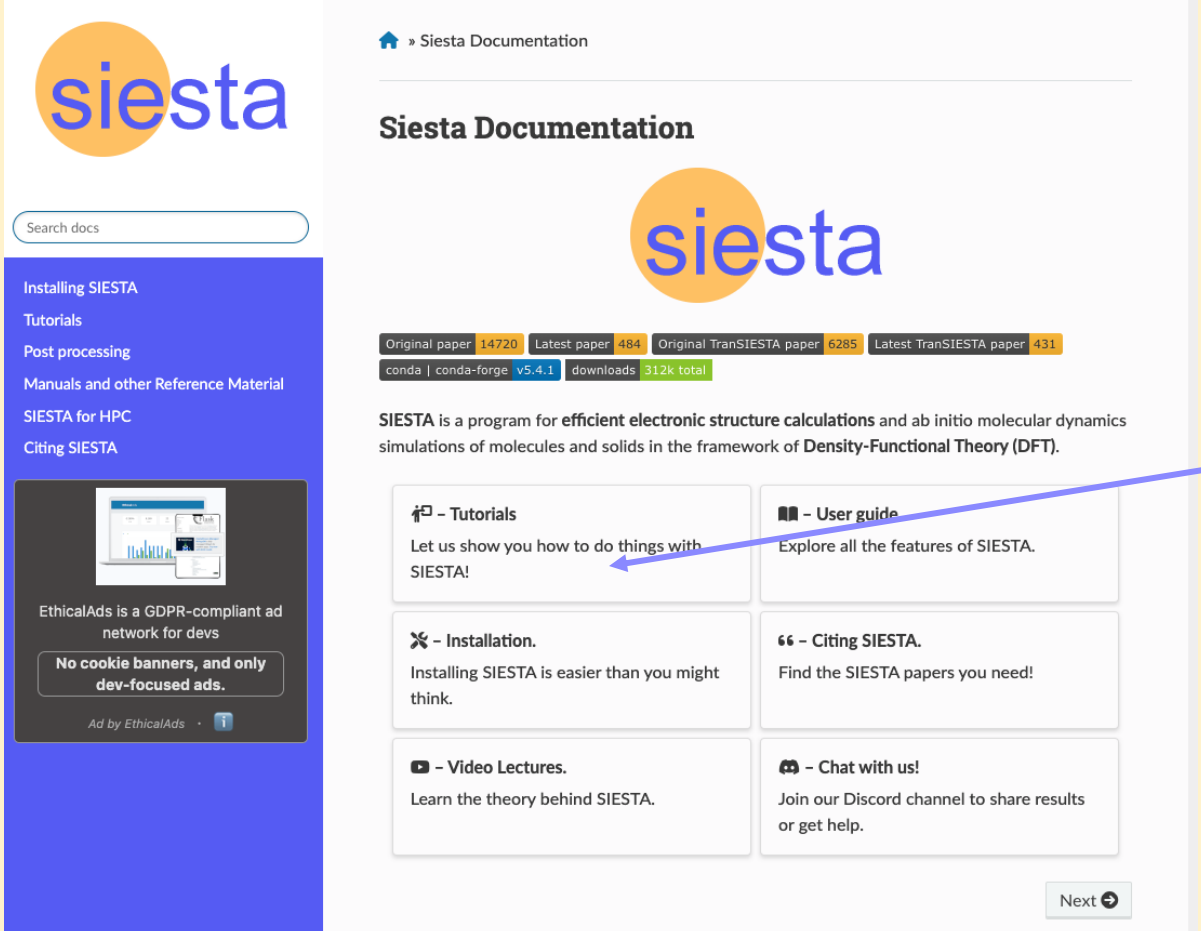
Please make sure that your CECAM account is up to date and uses your current email address.

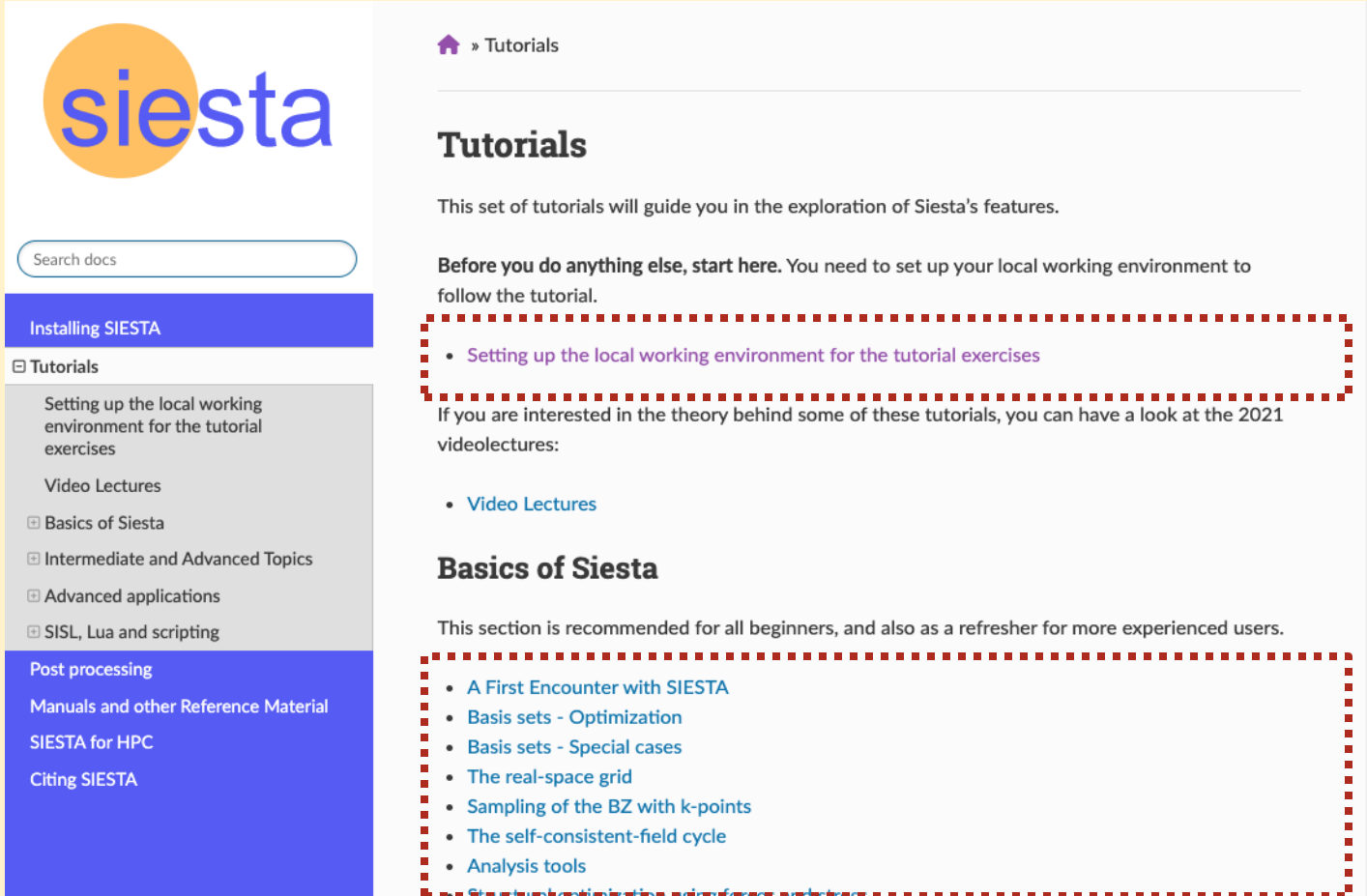
The deadline for applications is the **17th October 2025**.

We will review applications in stages and we will communicate all our acceptance decisions by email by the 24th October 2025. The names of all the accepted participants will appear on the participants tab of the CECAM website.

Siesta documentation site



Siesta documentation site



Repo with all the tutorials inputs

Basic tutorials

Before we begin…

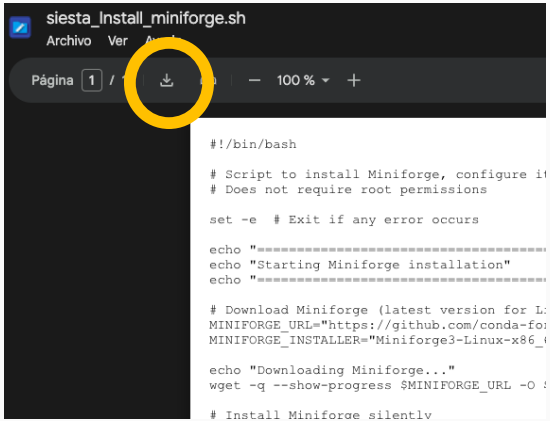
Were you able to install SIESTA with conda?

How many of you were able to do it?

Linux users

- Download the next script: **siesta_Install_miniforge.sh**

https://drive.google.com/file/d/11_1SOK51T7bwoKmwuIE_IwUrtO_zyAJL/view?usp=sharing



Downloads

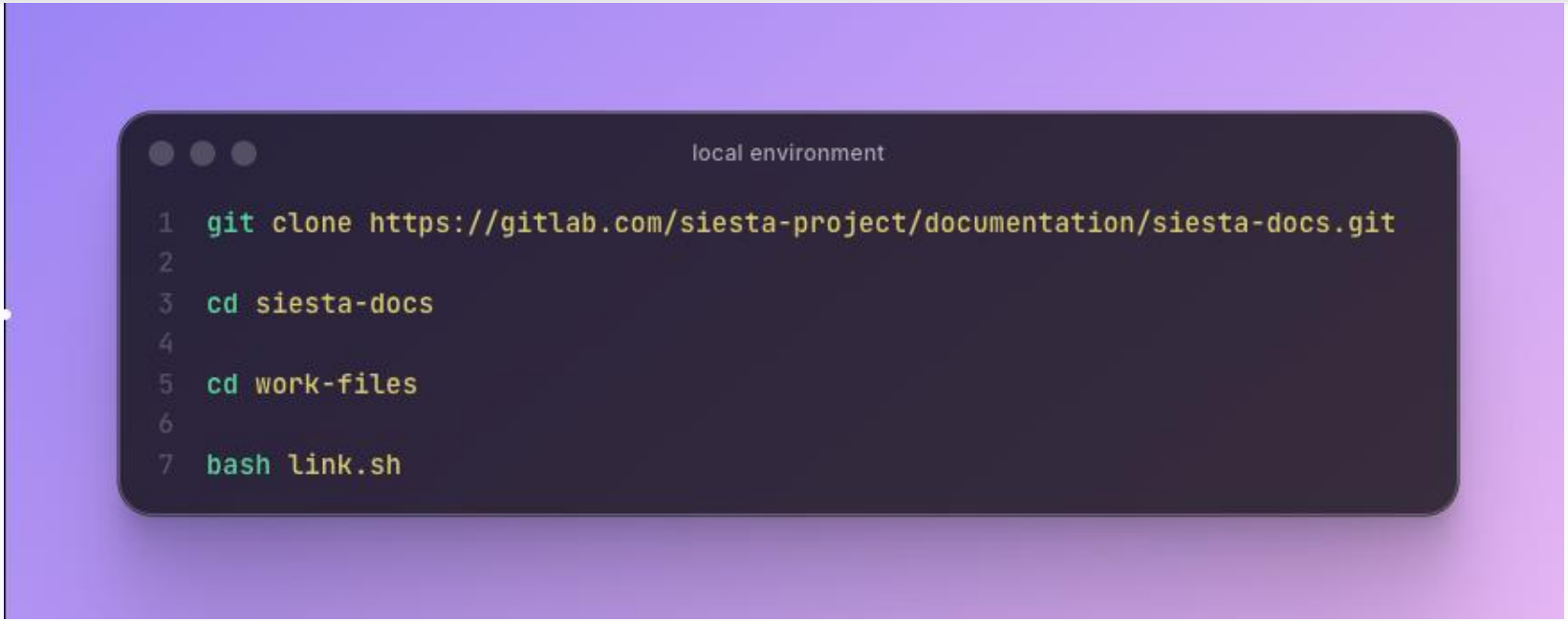
Linux users

- cp ~/Downloads/siesta_Install_miniforge.sh .
- Execute the bash script and it will install conda, create an environment for this school and, install siesta 5.4.1.

Linux users

```
==========================================
Installation completed successfully!
==========================================

Python version installed:
Python 3.14.0

To use the environment in the future, run:
  conda activate siesta_school

To verify SIESTA installation, run:
  siesta --version

Executable      : siesta
Version         : 5.4.1
Architecture    : x86_64
Compiler version: GNU-14.3.0
Compiler flags  : -march=nocona -mtune=haswell -ftree-vectorize -fPIC -fstack-protector-
env/include -fdebug-prefix-map=<prefix>/work=/usr/local/src/conda/siesta-5.4.1 -fdebug-p
3
Parallelisations: MPI
NetCDF support
NetCDF-4 support
NetCDF-4 MPI-IO support
Lua support
ELSI support. Solvers:
   ELPA (internal)
   NTPoly
   OMM
DFT-D3 support

SIESTA packages installed:
# packages in environment at /home/ICN2/aalcaraz/miniforge3/envs/siesta_school:
siesta                    5.4.1           mpi_openmpi_h7956b2f_0  conda-forge
==========================================
```

Setting up the local working environment for the tutorial exercises



How is the material organized?

siesta_school_my_workspace/

siesta-docs/

- **docs/**
- LICENSE
- README.md
- **work-files/**
  - link.sh
  - **tutorials/**
- **yaml_tests/**

tutorials/

- **advanced/**
- **applications/**
- **basic/**
  - **first-encounter/**
  - .../
  - .../
- **scripting/**

Remember which folder you are working in

Some tutorials may be updated during the week

siesta_school_my_workspace/

siesta-docs/ $ git pull

work-files/ $ bash link.sh

Pay attention to the instructions from each instructor.

How do we run  ?

Load de environment

commands

- Activate the conda environment:

conda activate siesta_school

- Verify siesta availability

which siesta

/home/ICN2/aalcaraz/miniforge3/envs/siesta_school/bin/siesta

siesta --version

```
Executable      : siesta
Version         : 5.4.1
Architecture    : x86_64
Compiler version: GNU-14.3.0
Compiler flags  : -march=nocona -mtune=haswell -ftree-
env/include -fdebug-prefix-map=<prefix>/work=/usr/loca
3
Parallelisations: MPI
NetCDF support
```

Exercise 1

Enter:

siesta_school_my_workspace/siesta-docs/work-files/tutorials/basic/first-encounter/01-CH4-Basic

```
first-encounter/
├── 01-CH4-Basic/
│   ├── ch4.fdf
│   ├── C.psml
│   └── H.psml
├── 02-CH4-Basis/
└── 03-CH4-XC-Functional/
```

```
first-encounter/
├── 01-CH4-Basic/
│   ├── ch4.fdf
│   ├── C.psml
│   ├── H.psml
│   └── exercise_1
│       ├── ch4.fdf
│       ├── C.psml
│       └── H.psml
```

- Create a new folder inside 01-CH4-Basic: **exercise_1**
- Copy the inputs from 01-CH4-BASIC to exercise_1
- Execute the following:

```
mkdir  exercise_1
cp ch4.fdf C.psml H.psml exercise_1/
cd exercise_1
```

First run

```
mpiexec -n 4 siesta ch4.fdf > ch4.out
```

What did this command do?

What are the main ingredients?

For most basic SIESTA calculations, we need at least **two** inputs:

- Pseudo potential files (e.g. available in PSML format from http://www.pseudo-dojo.org, or a PSF created with ATOM).
- An fdf file with the input options (Flexible Data Format).

```
exercise_1/
├── ch4.fdf
├── C.psml
└── H.psml
```

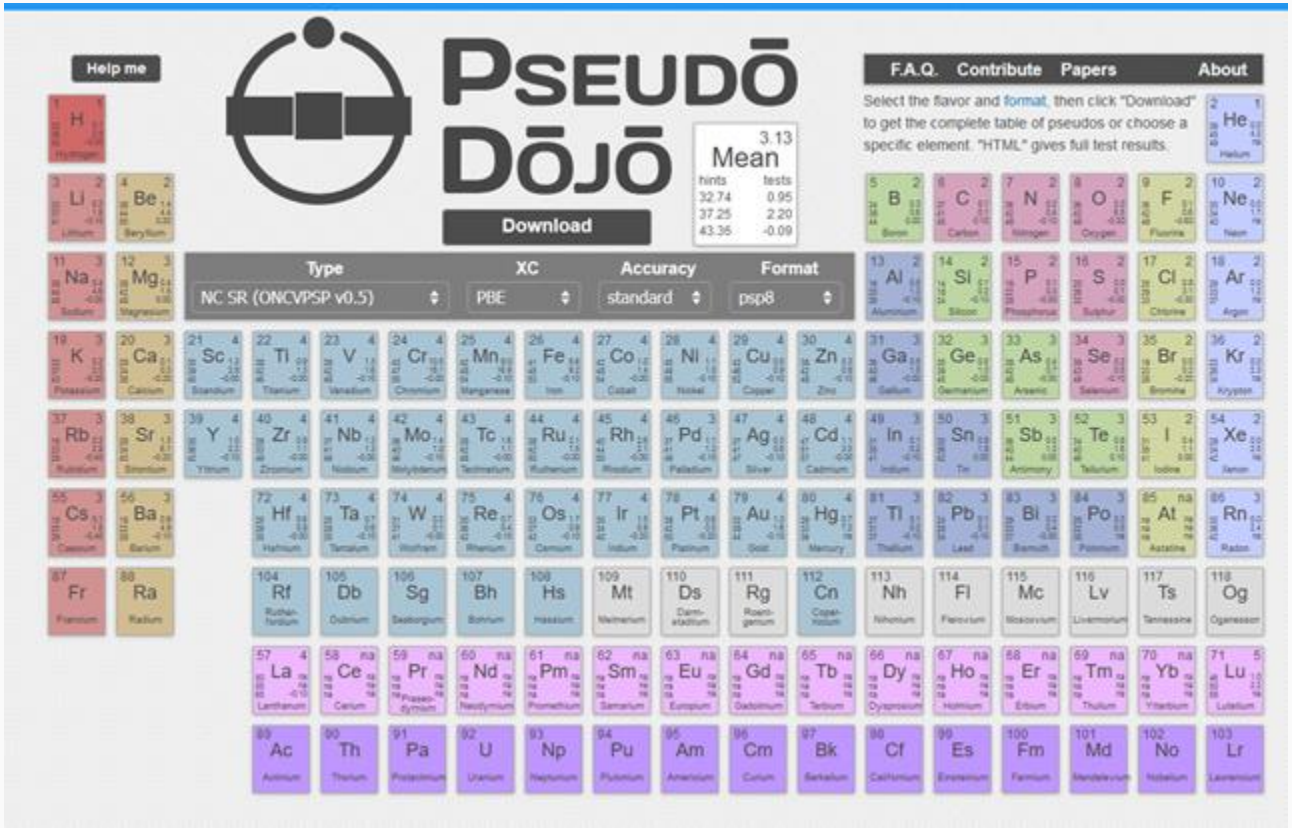
First run

```
mpiexec -n 4 siesta ch4.fdf > ch4.out
```

First ingredient: pseudopotential

Exercise 1

Recommended way: *get it from pseudo-dojo* (pseudo-dojo.org) *as a psml file.*



Second ingredient: What's in the FDF?

The fdf file contains all relevant input options for our simulation:

- Sort of data:
  - Name-value pairs
  - Blocks
- Case insensitive
- Minimal info:
  - General system information
  - Structural information

Let's have a look…

SystemLabel
NumberOfSpecies
NumberOfAtoms
ChemicalSpeciesLabel

LatticeConstant
LatticeVectors
AtomicCoordinatesFormat
AtomicCoordinatesAndAtomicSpecies

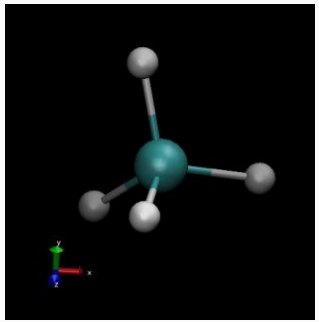
What's in the FDF? System information

```
#General system specifications
SystemName          CH4 molecule
SystemLabel         ch4
NumberOfAtoms       5
NumberOfSpecies     2

%block ChemicalSpeciesLabel
 1  6 C   # Species index, atomic number, species label
 2  1 H   # Species index, atomic number, species label
%endblock ChemicalSpeciesLabel
```

All output filenames will begin with "ch4."

Total number of atoms in the simulation box.

Different "kinds" of atoms present.



Note that we have to types of inputs: single variables, and blocks.

What's in the FDF? System geometry

```
#Unit cell for the calculation
LatticeConstant 15 Ang
%block LatticeVectors
  1.000 0.000 0.000
  0.000 1.000 0.000
  0.000 0.000 1.000
%endblock LatticeVectors
```

Multiplies all lattice vectors by a constant. Note the units.

The lattice vectors themselves.

```
#Atomic coordinates
AtomicCoordinatesFormat  Ang

%block AtomicCoordinatesAndAtomicSpecies
  0.000      0.000      0.000   1   # C
  1.219     -0.284     -0.377   2   # H
 -0.284      1.219     -0.377   2   # H
 -0.140     -0.140      1.219   2   # H
 -0.833     -0.833     -0.503   2   # H
%endblock AtomicCoordinatesAndAtomicSpecies
```

Unit for the atomic coordinates block. Can also be "fractional".

Atomic coordinates and species index (1 for C, 2 for H).

What's in the FDF? Other options

```
# Type of solution
SolutionMethod diagon

# Basis set definition
PAO.BasisSize   SZ
PAO.EnergyShift 250 meV

#Real space grid
MeshCutoff 125.0 Ry

# Convergence of SCF
MaxSCFIterations   50
SCF.Mixer.Weight   0.4
SCF.Mixer.History  2
```

Solver options.

Basis Set Options

Relates to the amount of points for grid-based operations.

Options for SCF acceleration.

What about the outputs?

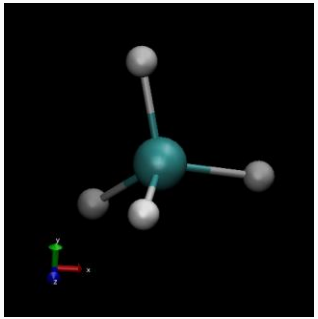
First run

```
mpiexec -n 4 siesta ch4.fdf > ch4.out
```

SIESTA prints out to standard output

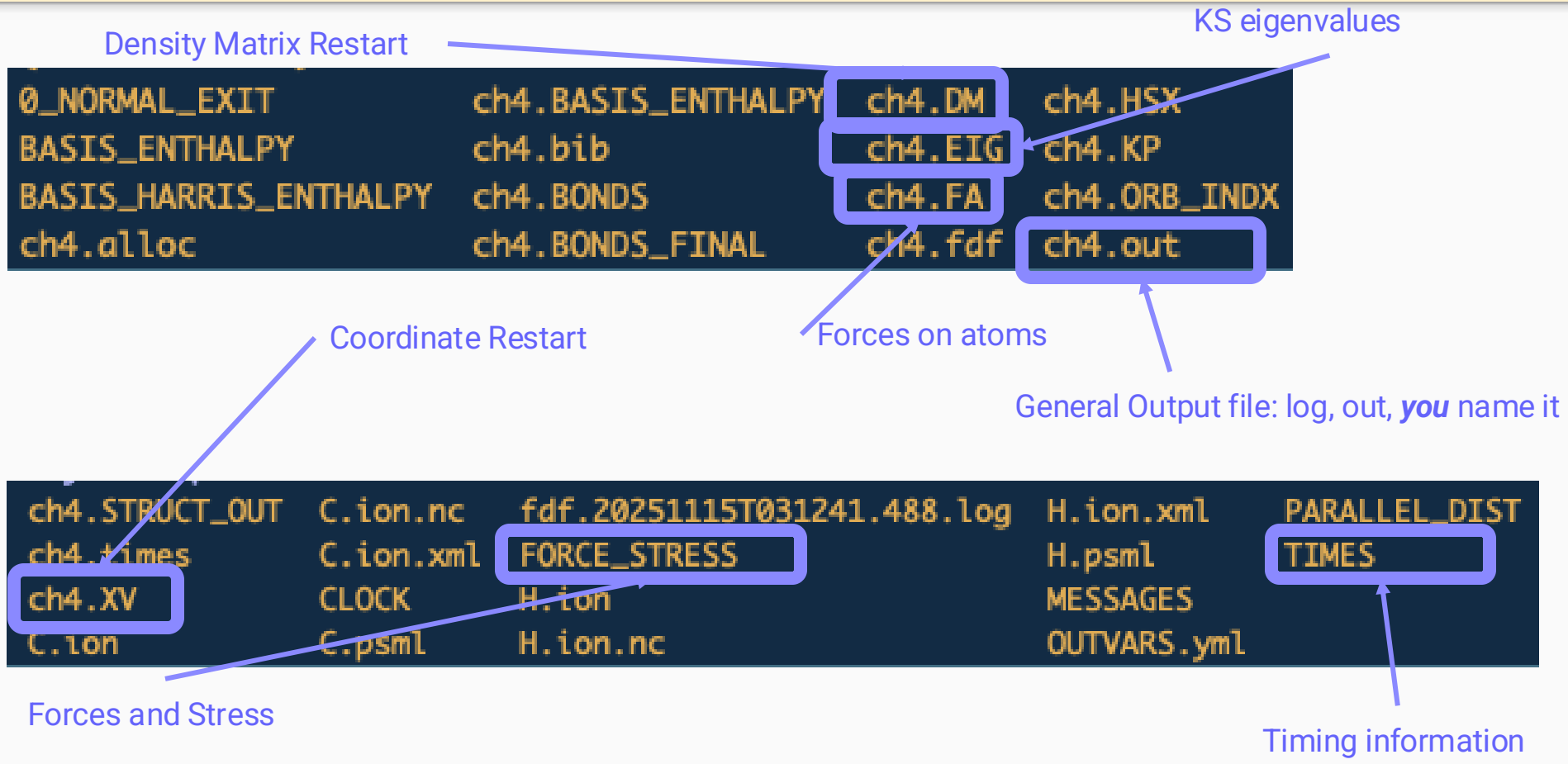
What are all of these files???

```
0_NORMAL_EXIT            ch4.BASIS_ENTHALPY   ch4.DM    ch4.HSX
BASIS_ENTHALPY           ch4.bib              ch4.EIG   ch4.KP
BASIS_HARRIS_ENTHALPY    ch4.BONDS            ch4.FA    ch4.ORB_INDX
ch4.alloc                ch4.BONDS_FINAL      ch4.fdf   ch4.out
```



```
ch4.STRUCT_OUT   C.ion.nc   fdf.20251115T031241.488.log   H.ion.xml     PARALLEL_DIST
ch4.times        C.ion.xml  FORCE_STRESS                  H.psml        TIMES
ch4.XV           CLOCK      H.ion                         MESSAGES
C.ion            C.psml     H.ion.nc                      OUTVARS.yml
```

What are all of these files???



Outputs: ch4.out

Installation and run info, Start Time

```
Executable      : siesta
Version         : unreleased a05b5f95a (2025-09-16)
Architecture    : x86_64
Compiler version: GNU-13.3.0
Compiler flags  : -fallow-argument-mismatch -O3 -march=native
Parallelisations: MPI
Lua support
ELSI support. Solvers:
   ELPA (internal)
   NTPoly
   OMM
DFT-D3 support

Runtime information:
* Directory : /users/ens/alcaraza/Siesta/siesta-docs/work-files/tutorials/basic/first-encounter/01-CH4-Basic
* Running on 4 nodes in parallel.
>> Start of run:  29-OCT-2025  17:43:57

                           ***********************
                           *  WELCOME TO SIESTA  *
                           ***********************
```

Outputs

```
initatom: Reading input for the pseudopotentials and atomic orbitals ----------
Species number:   1 Atomic number:    6 Label: C
Species number:   2 Atomic number:    1 Label: H

Ground state valence configuration (from tables):   2s02  2p02  3d00  4f00
Ground state valence configuration (from tables):   1s01  2p00  3d00  4f00

---- Processing specs for species: C
Reading pseudopotential information in PSML from:
  C.psml
PSML file version: 1.1
Using libxc ids:  116 133
GGA--PBEsol XC_GGA_X_PBE_SOL--XC_GGA_C_PBE_SOL ps
PSML uuid: 51a02af0-1d5f-11e8-49c3-12b9ebd99919

---- Processing specs for species: H
Reading pseudopotential information in PSML from:
  H.psml
PSML file version: 1.1
Using libxc ids:    1  12
LDA--PW92 XC_LDA_X--XC_LDA_C_PW pw
PSML uuid: c4d96a40-23d1-11e8-69b6-c18eff5d81ce

---- Pseudopotential check for C

Pseudized shells:
2s( 2.00) rc: 1.20
2p( 2.00) rc: 1.26
Valence configuration for ps generation: 2s:2p: Total charge:   4.000000

---- Pseudopotential check for H

Pseudized shells:
1s( 1.00) rc: 1.01
2p( 0.00) rc: 0.91
Valence configuration for ps generation: 1s: Total charge:   1.000000
For C, standard SIESTA heuristics set lmxkb to 2
 (one more than the basis l, including polarization orbitals).
Use PS.lmax or PS.KBprojectors blocks to override.
```

Species and pseudopotential information

Outputs

```
atom: ---------------------------------------------------------------------

atom: SANKEY-TYPE ORBITALS:

SPLIT: Orbitals with angular momentum L= 0

SPLIT: Basis orbitals for state 2s

SPLIT: PAO cut-off radius determined from an
SPLIT: energy shift=  0.018375 Ry
Split based on tail norm

   izeta = 1
                 lambda =    1.000000
                     rc =    4.188930
                 energy =   -0.981019
                kinetic =    0.980783
    potential(screened) =   -1.961802
       potential(ionic) =   -5.541734

SPLIT: Orbitals with angular momentum L= 1

SPLIT: Basis orbitals for state 2p

SPLIT: PAO cut-off radius determined from an
SPLIT: energy shift=  0.018375 Ry
Split based on tail norm

   izeta = 1
                 lambda =    1.000000
                     rc =    4.967013
                 energy =   -0.365210
                kinetic =    2.559078
    potential(screened) =   -2.924288
       potential(ionic) =   -6.383934
atom: Total number of Sankey-type orbitals:  4

atm_pop: Valence configuration (for local Pseudopot. screening):
 2s( 2.00)
 2p( 2.00)
Vna: chval, zval:    4.00000   4.00000
```

Basis set generation

Outputs

Coordinates and selected options

```
coor:   Atomic-coordinates input format  =     Cartesian coordinates
coor:                                          (in Angstroms)

siesta: Atomic coordinates (Bohr) and species
siesta:      0.00000   0.00000   0.00000  1       1
siesta:      2.30358  -0.53668  -0.71243  2       2
siesta:     -0.53668   2.30358  -0.71243  2       3
siesta:     -0.26456  -0.26456   2.30358  2       4
siesta:     -1.57414  -1.57414  -0.95053  2       5

siesta: System type = molecule

initatomlists: Number of atoms, orbitals, and projectors:      5     8    28

siesta: ****************** Simulation parameters ***************************
siesta:
siesta: The following are some of the parameters of the simulation.
siesta: A complete list of the parameters used, including default values,
siesta: can be found in file out.fdf
siesta:
redata: Spin configuration                          = none
redata: Number of spin components                   = 1
redata: Time-Reversal Symmetry                      = T
redata: Spin spiral                                 = F
redata: Long output                                 =   F
redata: Number of Atomic Species                    =       2
redata: Charge density info will appear in .RHO file
redata: Write Mulliken charges (when)               = none
redata: Write Mulliken Pop.                         = NO
redata: Write Hirshfeld charges (when)              = none
redata: Write Voronoi charges (when)                = none
redata: Write spin charge (when)                    = none
redata: Matel table size (NRTAB)                    =     1024
redata: Mesh Cutoff                                 =   125.0000 Ry
redata: Net charge of the system                    =     0.0000 |e|
redata: Min. number of SCF Iter                     =        0
redata: Max. number of SCF Iter                     =       50
redata: SCF convergence failure will abort job
redata: SCF mix quantity                            = Hamiltonian
redata: Mix DM or H after convergence               =   F
redata: Recompute H after scf cycle                 =   F
```

Outputs

```
                     ============================
                        Single-point calculation
                     ============================

outcell: Unit cell vectors (Ang):
       15.000000    0.000000    0.000000
        0.000000   15.000000    0.000000
        0.000000    0.000000   15.000000

outcell: Cell vector modules (Ang)   :   15.000000   15.000000   15.000000
outcell: Cell angles (23,13,12) (deg):     90.0000     90.0000     90.0000
outcell: Cell volume (Ang**3)        :   3375.0000
<dSpData1D:S at geom step 0
  <sparsity:sparsity for geom step 0
    nrows_g=8 nrows=2 sparsity=.2500 nnzs=16, refcount: 7>
  <dData1D:(new from dSpData1D) n=16, refcount: 1>
refcount: 1>
new_DM -- step:     1
Initializing Density Matrix...

Attempting to read DM from file... Failed...
DM filled with atomic data:
<dSpData2D:DM initialized from atoms
  <sparsity:sparsity for geom step 0
    nrows_g=8 nrows=2 sparsity=.2500 nnzs=16, refcount: 8>
  <dData2D:DM n=16 m=1, refcount: 1>
refcount: 1>
No. of atoms with KB's overlaping orbs in proc 0. Max # of overlaps:       5       8

InitMesh: MESH = 108 x 108 x 108 = 1259712
InitMesh: Mesh cutoff (required, used) =   125.000   143.274 Ry
New grid distribution [1]: sub = 2
New grid distribution [2]: sub = 2
New grid distribution [3]: sub = 2
Setting up quadratic distribution...

stepf: Fermi-Dirac step function

siesta: Program's energy decomposition (eV):
siesta: Ebs     =       -87.057890
```

Type of run, cell information.

Sparsity information.

Mesh information.

Outputs

```
siesta: Program's energy decomposition (eV):
siesta: Ebs     =       -87.057890
siesta: Eions   =       407.435544
siesta: Ena     =       134.583366
siesta: Ekin    =       143.164339
siesta: Enl     =       -10.642485
siesta: Eso     =         0.000000
siesta: Edftu   =         0.000000
siesta: DEna    =         3.582210
siesta: DUscf   =         0.299525
siesta: DUext   =         0.000000
siesta: Ex      =       -74.401564
siesta: Ec      =       -11.671706
siesta: Exc     =       -86.073270
siesta: EbV     =         0.000000
siesta: eta*DQ  =         0.000000
siesta: Emadel  =         0.000000
siesta: Emeta   =         0.000000
siesta: Emolmec =         0.000000
siesta: Ekinion =         0.000000
siesta: Eharris =      -232.130754
siesta: Etot    =      -222.521860
siesta: FreeEng =      -222.521860
```

Initial, non-SCF energy decomposition.

Outputs

```
      iscf     Eharris(eV)        E_KS(eV)     FreeEng(eV)     dDmax    Ef(eV) dHmax(eV)
   scf:    1     -232.130754     -222.521860     -222.521860  1.101199 -6.841474  1.028330
timer: Routine,Calls,Time,% = IterSCF        1       0.155  24.53
   scf:    2     -222.542289     -222.538095     -222.538095  0.022736 -6.524821  0.232074
   scf:    3     -222.538153     -222.538197     -222.538197  0.002707 -6.429279  0.141576
   scf:    4     -222.538205     -222.538216     -222.538216  0.001493 -6.290235  0.047798
   scf:    5     -222.538224     -222.538221     -222.538221  0.000478 -6.324841  0.001216
   scf:    6     -222.538221     -222.538221     -222.538221  0.000031 -6.324150  0.000384

SCF Convergence by DM+H criterion
max |DM_out - DM_in|         :     0.0000305952
max |H_out - H_in|      (eV) :     0.0003842923
SCF cycle converged after 6 iterations

Using DM_out to compute the final energy and forces
No. of atoms with KB's overlaping orbs in proc 0. Max # of overlaps:      5      8

siesta: E_KS(eV) =             -222.5382

siesta: E_KS - E_eggbox =      -222.5382

siesta: Atomic forces (eV/Ang):
----------------------------------------
   Tot    0.002408    0.002408   -0.001498
----------------------------------------
   Max    2.338422
   Res    1.118414    sqrt( Sum f_i^2 / 3N )
----------------------------------------
   Max    2.338422    constrained

Stress tensor Voigt[x,y,z,yz,xz,xy] (kbar):       1.98       1.98       0.92      -0.21      -0.21      -0.03
(Free)E + p*V (eV/cell)     -225.9574
Target enthalpy (eV/cell)     -222.5382
```

SCF cycle information

Converged KS energy

Converged total forces and cell stress

Outputs

Final energy decomposition

```
siesta: Program's energy decomposition (eV):
siesta: Ebs     =       -88.949134
siesta: Eions   =       407.435544
siesta: Ena     =       134.583366
siesta: Ekin    =       141.825781
siesta: Enl     =       -10.477008
siesta: Eso     =         0.000000
siesta: Edftu   =         0.000000
siesta: DEna    =         4.466002
siesta: DUscf   =         0.266389
siesta: DUext   =         0.000000
siesta: Ex      =       -74.112598
siesta: Ec      =       -11.654609
siesta: Exc     =       -85.767207
siesta: EbV     =         0.000000
siesta: eta*DQ  =         0.000000
siesta: Emadel  =         0.000000
siesta: Emeta   =         0.000000
siesta: Emolmec =         0.000000
siesta: Ekinion =         0.000000
siesta: Eharris =      -222.538221
siesta: Etot    =      -222.538221
siesta: FreeEng =      -222.538221

siesta: Final energy (eV):
siesta:  Band Struct. =     -88.949134
siesta:       Kinetic =     141.825781
siesta:       Hartree =     282.961698
siesta:         Edftu =       0.000000
siesta:       Eso     =       0.000000
siesta:    Ext. field =       0.000000
siesta:         Exch. =     -74.112598
siesta:         Corr. =     -11.654609
siesta:     Bulk bias =       0.000000
siesta:   Exch.-corr. =     -85.767207
siesta:  Ion-electron =    -696.354718
siesta:       Ion-ion =     134.796225
siesta:       Ekinion =       0.000000
siesta: D3 dispersion =       0.000000
siesta:         Total =    -222.538221
siesta:         Fermi =      -6.324150
```

Outputs

Final forces

Final stress/pressure

Electric dipole

```
siesta: Atomic forces (eV/Ang):
siesta:      1    0.164966    0.164966   -1.084421
siesta:      2   -2.338422    0.480063    0.757120
siesta:      3    0.480063   -2.338422    0.757120
siesta:      4    0.338967    0.338967   -0.916986
siesta:      5    1.356834    1.356834    0.485668
siesta: ----------------------------------------
siesta:    Tot    0.002408    0.002408   -0.001498

siesta: Stress tensor (static) (eV/Ang**3):
siesta:     0.001233   -0.000021   -0.000128
siesta:    -0.000021    0.001233   -0.000128
siesta:    -0.000128   -0.000128    0.000572

siesta: Cell volume =       3375.000000 Ang**3

siesta: Pressure (static):
siesta:                Solid           Molecule  Units
siesta:          -0.00001103          0.00000000  Ry/Bohr**3
siesta:          -0.00101308          0.00000045  eV/Ang**3
siesta:          -1.62314011          0.00072877  kBar

Basis Enthalpy Calculation:
    Basis Pressure for species 1(C) :      0.2000000 GPa
    Basis Pressure for species 2(H) :      0.2000000 GPa

    Orbital volume contribution        =          0.496873 eV
    (Free)E + p_basis*V_orbitals       =       -222.041348 eV
    (Free)Eharris+ p_basis*V_orbitals  =       -222.041349 eV
WARNING: BASIS_ENTHALPY and BASIS_HARRIS_ENTHALPY files are deprecated. They will be removed in future releases.
Please use system_label.BASIS_ENTHALPY in your scripts instead.

siesta: Electric dipole (a.u.)  =   -0.011465   -0.011465    0.009499
siesta: Electric dipole (Debye) =   -0.029140   -0.029140    0.024144
```

Outputs

Primary bibliography, and end-of-run time

```
cite: Please indicate the Siesta version in published work: unreleased a05b5f95a (2025-09-16)
cite: This calculation has made use of features in the following articles
cite: which we encourage you to cite in published work.
cite: (Please see "ch4.bib" for a BibTeX file.)
       Primary SIESTA paper
         DOI: www.doi.org/10.1088/0953-8984/14/11/302
       PSML pseudopotential format
         DOI: www.doi.org/10.1016/j.cpc.2018.02.011


>> End of run:  29-OCT-2025  17:43:59
Job completed
```

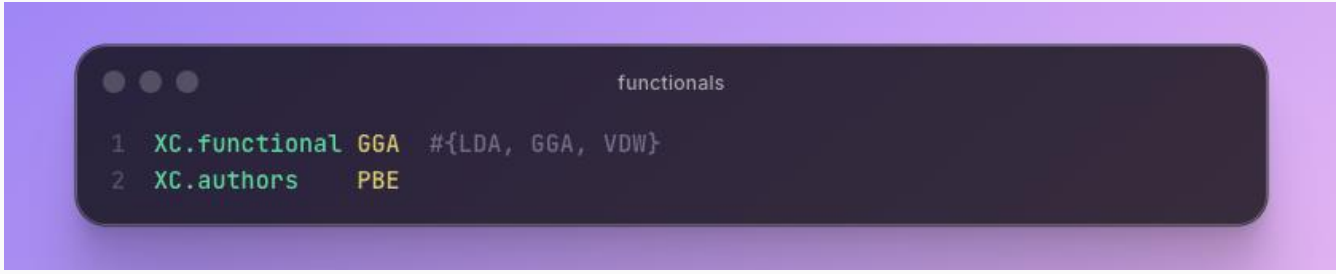
Other things to choose

1. Pseudopotentials
2. Functional
3. Basis set

Choosing a DFT functional

SIESTA offers different families of DFT functionals:

- LDA (CA, PW92)
- GGA (PW91,BLYP, PBE, PBESol, RevPBE)
- Van der Waals functionals (DRSLL, VV)



A peek into basis sets

For now, we will only concern ourselves with:

- Exploring the basis set cardinality (SZ,DZ, SZP, DZP,TZP), i.e. *the amount of basis functions per atom*. In principle, more functions imply a better quality, but also an increase in computational costs.

- Playing with the *energy shift*, which essentially modifies the cut-off radius of the basis set. The lower the energy shift, the larger the cut-off radius of the orbitals.

Exercise 2 (We will improve our input)

Enter:

siesta_school_my_workspace/siesta-docs/work-files/tutorials/basic/first-encounter/02-CH4-Basis

```
first-encounter/
├── 01-CH4-Basic/
├── 02-CH4-Basis/
│   ├── ch4.fdf
│   ├── C.psml
│   └── H.psml
└── 03-CH4-XC-Functional/
```

```
first-encounter/
├── 02-CH4-Basis /
│   ├── ch4.fdf
│   ├── C.psml
│   ├── H.psml
│   └── exercise_2
```

- Create a new folder inside 02-CH4-Basis: **exercise_2**

mkdir exercise_2

Exercise 2 (We will improve our input)

INPUTS FOLDER

```
../
├── 02-CH4-Basis/
```

exercise folder

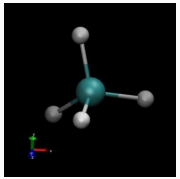
```
02-CH4-Basis/
├──── exercise_2/
│   ├──── SZ_10
│   ├──── SZ_50
```

1. Copy all files from the input folder to the each condition folder.
2. In this exercise you will do a scan modifying the basis set and the energy shift value.

```
# Basis set definition
PAO.BasisSize   SZ
PAO.EnergyShift 250 meV
```

SZ DZ SZP DZP TZP

Energy Shifts (meV): 10 50 100 150 200 250 300



Everything depends on how you organize it

siesta: Total = -221.815381

Exercise 2 (We will improve our input)

INPUTS FOLDER

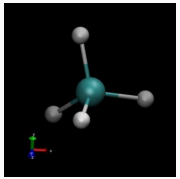
```
../
├── 02-CH4-Basis/
```

exercise folder

```
02-CH4-Basis/
├──── exercise_2/
|   ├──── SZ_10
|   ├──── SZ_50
```

- You will need to extract the total energy from each output file for every tested condition
- Generate a data file for each tested basis.

Energy file for SZ



```
#E. Shift        Total Energy
#   [meV]           [eV]
#_____________________________
10              -221.815381
50              -221.815381
100             -221.815381
150             -221.815381
200             -221.815381
250             -221.815381
300             -221.815381
```

You will have 5 files with the energy info.

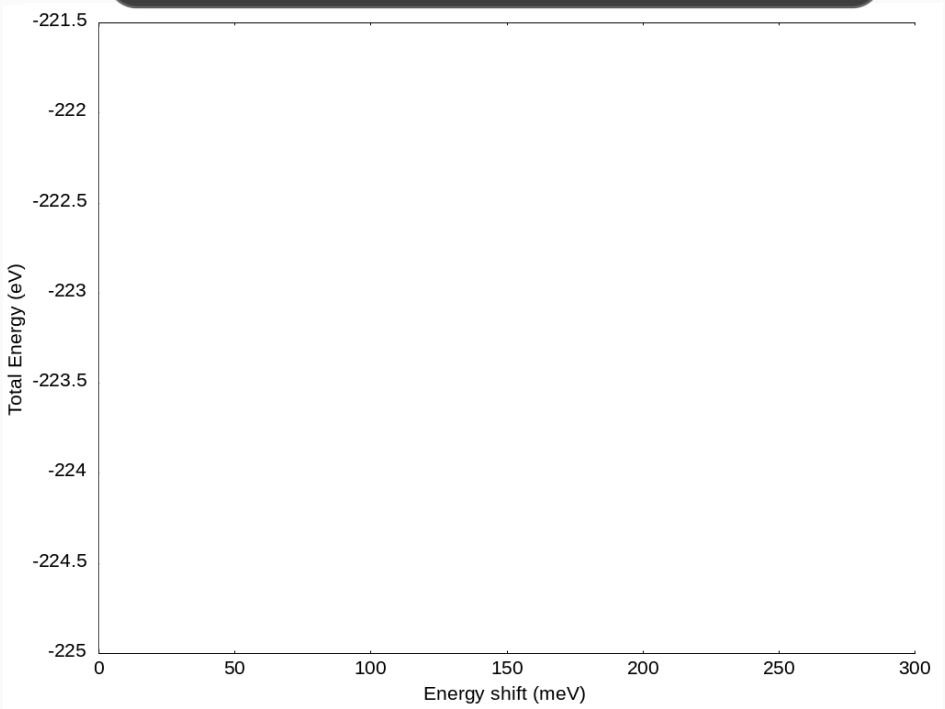
Exercise 2 (We will improve our input)

https://drive.google.com/file/d/1azhV9PiwxDUYJvdd72aD4nogV3RyQQfS/view?usp=sharing

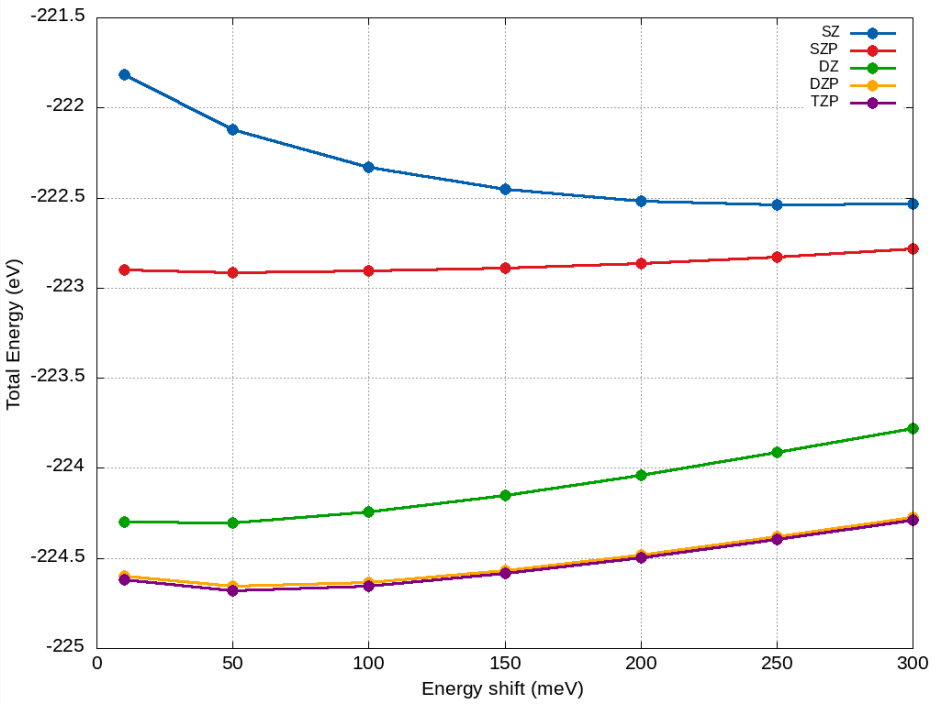
../
├── plot_gnuplot.sh

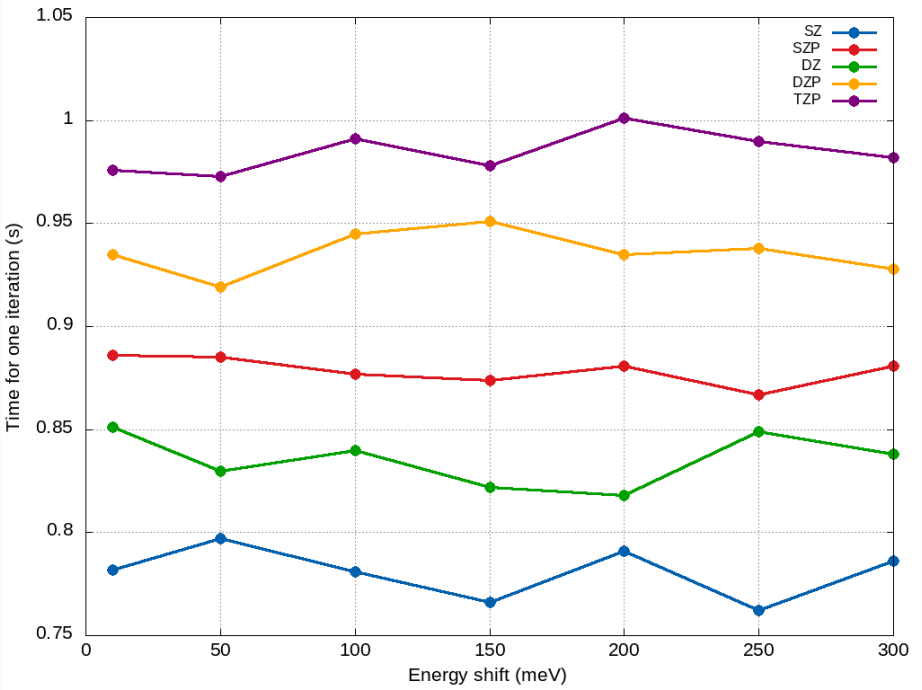
Basis set

```
bash ../siesta/plot_gnuplot.sh -x "Energy shift (meV)" \
-y "Total Energy (eV)" -l "SZ, SZP, DZ, DZP, TZP" \
-f bes_1.dat bes_2.dat bes_3.dat bes_4.dat bes_5.dat
```



Exercise 2 (We will improve our input)





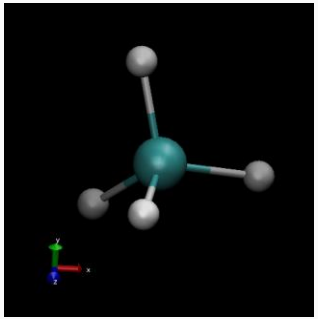
Exercise 2

(Best options for CH_4)

```
# Basis set definition
PAO.BasisSize   SZ
PAO.EnergyShift 250 meV
```

DZP

50-100 meV



Exercise 3

Enter:

siesta_school_my_workspace/siesta-docs/work-files/tutorials/basic/first-encounter/03-CH4-XC-Functional

```
first-encounter/
├── 01-CH4-Basic/
├── 02-CH4-Basis/
├── 03-CH4-XC-Functional/
│   ├── ch4.fdf
│   ├── C.psml
│   ├── H.psml
│   ├── C.gga.psml
│   └── H.gga.psml
```

```
first-encounter/
├── 03-CH4-XC-Functional/
│   ├── ch4.fdf
│   ├── C.psml
│   ├── H.psml
│   ├── C.gga.psml
│   ├── H.gga.psml
│   └── exercise_3
```

- Create a new folder inside 03-CH4-XC-Functional: **exercise_3**
- Copy the 4 pseudopotentials and the FDF file to exercise_3

```
mkdir  exercise_3
cp *.psml ch4.fdf exercise_3
```

Exercise 3

Enter:

siesta_school_my_workspace/siesta-docs/work-files/tutorials/basic/first-encounter/03-CH4-XC-Functional

- Modify these lines in the input file and execute the job:

03-CH4-XC-Functional

```
XC.functional GGA
XC.authors    PBE
```

03-CH4-XC-Functional

```
mpiexec -n 4 siesta ch4.fdf > ch4.out
```

- You will find the following warning in the output

```
xc_check: Exchange-correlation functional:
xc_check: GGA Perdew, Burke & Ernzerhof 1996
xc_check: WARNING: Pseudopotential generated with LDA PW92 functional
Got Vlocal (oncv-fit) from psml data
Choosing vlocal chloc cutoff:  1.752670
qtot up to nchloc:    1.00000855
```

Exercise 4

Enter:

siesta_school_my_workspace/siesta-docs/work-files/tutorials/basic/first-encounter/03-CH4-XC-Functional

- Create a new folder (exercise 4), copy the inputs from the parent folder and modify the input:

Did you get the warning?

Exercise 4

Enter:

siesta_school_my_workspace/siesta-docs/work-files/tutorials/basic/first-encounter/03-CH4-XC-Functional

```
xc_check: Exchange-correlation functional:
xc_check: GGA Perdew, Burke & Ernzerhof 1996
xc_check: WARNING: Pseudopotential generated with GGA PBEsol functional
Got Vlocal (oncv-fit) from psml data
Choosing vlocal chloc cutoff:  4.114026
qtot up to nchloc:    4.00001066
```

Did you get the warning?

Exercise 5

Enter:

siesta_school_my_workspace/siesta-docs/work-files/tutorials/basic/first-encounter/03-CH4-XC-Functional

- Create a new folder (exercise 5), copy the inputs from the parent folder and modify the input:
- Modify the XC.Authors and run again. Did you get the warning?

```
xc_check: Exchange-correlation functional:
xc_check: GGA PBEsol
Got Vlocal (oncv-fit) from psml data
Choosing vlocal chloc cutoff:  4.114026
```

Questions?