

A first encounter with TM

11/11/2024 - Federico Pedron



How do we run  siesta?
TM

Reminder: how to connect

https://siesta-project.org/siesta/events/SIESTA_School-2024/MN5.html

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https://siesta-project.org/siesta/events/SIESTA_School-2024/MN5.html

ssh nct01YYY@glogin1.bsc.es

Where **YYY** is a number unique to each of you (001, 008, 017, 035, 079).

Use also **glogin2!** (only for data/password: **transfer1.bsc.es**)

Reminder: tutorial files

Each day, you should copy the tutorial folder available at
`/gpfs/projects/nct_315/TUTORIALS/dayX`

For example:

```
cp -r /gpfs/projects/nct_315/TUTORIALS/day1 day1
```

Submitting a job

In each run folder, copy the sample run script from
`/gpfs/projects/nct_315/SCRIPTS/runmn.sh`

```
cp /gpfs/projects/nct_315/SCRIPTS/runmn.sh 1-FirstEncounter/.
```

Submitting a job

Edit the run script!

```
#!/bin/bash
#SBATCH -J tutorialXX
#SBATCH -n 4
#SBATCH -t 0:30:00
#SBATCH -o %x-%j.out
#SBATCH -e %x-%j.err
#SBATCH -q gp_training
#SBATCH -A nct_315
#SBATCH -D .
##
## Uncomment the following line, change X by the current day of the school (1-5)
##SBATCH --reservation=SIESTA24-DAY1X

# DO NOT CHANGE THIS LINE
source /gpfs/projects/nct_315/SIESTA/siestarc.sh

# EDIT TO ADD THE CORRECT INPUT AND OUTPUT FILES.
srun -n 4 siesta < input.fdf > output.out
```

Submitting a job

Edit the run script!

```
#!/bin/bash
#SBATCH -J tutorialXX
#SBATCH -n 4
#SBATCH -t 0:30:00
#SBATCH -o %x-%j.out
#SBATCH -e %x-%j.err
#SBATCH -q gp_training
#SBATCH -A nct_315
#SBATCH -D .
##
## Uncomment the following line, change X by the current day of the school (1-5)
##SBATCH --reservation=SIESTA24-DAY1X

# DO NOT CHANGE THIS LINE
source /gpfs/projects/nct_315/SIESTA/siestarc.sh

# EDIT TO ADD THE CORRECT INPUT AND OUTPUT FILES.
srun -n 4 siesta < input.fdf > output.out
```


Submitting a job

Submit!

```
sbatch runmn.sh
```

To use reservations (from 12:00 to 19:00 CET) :

```
sbatch runmn.sh --reservation=SIESTA24-DAY1X (X=1,2,3,4,5)
```

https://siesta-project.org/siesta/events/SIESTA_School-2024/MN5.html

A look at the inputs

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.

What's in the FDF?

The fdf file contains all relevant input options for our simulation: geometry information, atomic species information, level of theory, basis set information, and a plethora of fine-tuning options.

Let's have a look at the first fdf for this tutorial...

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 two 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
```

```
#Atomic coordinates
```

```
AtomicCoordinatesFormat Ang
```

```
%block AtomicCoordinatesAndAtomicSpecies
```

```
0.000 0.000 0.000 1
```

```
1.219 -0.284 -0.377 2
```

```
-0.284 1.219 -0.377 2
```

```
-0.140 -0.140 1.219 2
```

```
-0.833 -0.833 -0.503 2
```

```
%endblock AtomicCoordinatesAndAtomicSpecies
```

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

The lattice vectors themselves.

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

```
# Basis set definition
PAO.EnergyShift 250 meV
PAO.SplitNorm 0.15
PAO.BasisSize SZ
```

Basis Set Options

```
#Real space grid
MeshCutoff 125.0 Ry
```

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

```
# Convergence of SCF
MaxSCFIterations 50
DM.MixingWeight 0.4
DM.NumberPulay 2
```

Options for SCF acceleration.

```
# Type of solution
SolutionMethod diagon
```

Solver options.

Let's try it!

Reminders

TUTORIAL:

<https://docs.siesta-project.org/projects/siesta/en/latest/tutorials/basic/first-encounter/index.html> (skip the last part)

- 1) `ssh nct01YYY@glogin2.bsc.es` ← (also `glogin1`)
- 2) `cp -r /gpfs/projects/nct_315/TUTORIALS/day1 .`
- 3) `cd day1/01.FirstEncounter`
- 4) `cp /gpfs/projects/nct_315/SCRIPTS/runmn.sh .`
- 5) (move and edit `runmn.sh` to your run folders)
- 6) `sbatch runmn.sh`

A First Encounter - Part 1: Running SIESTA

In this exercise we will get a first acquaintance with **SIESTA** by studying two simple molecules, CH₄ and CH₃. We will cover quite a lot of features and concepts, without worrying too much about issues of convergence.

Have you set up the local environment?

If not, [do that now](#) before proceeding.

The input files - fdf

Hint

Enter the directory 'first-encounter'

You will find an input file named `ch4.fdf`, along with the files `C.psf` and `H.psf` which contain the information about the pseudopotentials. The FDF (Flexible Data Format) file is the core input in

Let's have a look at the outputs...

Installation and run info, Start Time

```
Architecture      : ----
Compiler version: GNU-11.3.0
Compiler flags    : -fallow-argument-mismatch;-O3 -march=native
PP flags          : ----
Libraries         : ----
Parallelisations: MPI
GEMM3M support
NetCDF support
NetCDF-4 support
Lua support

Runtime information:
* Directory : /home/fnpedron/siesta-docs/work-files/tutorials/basic/first-encounter/CH4
* Running on 4 nodes in parallel.
>> Start of run:  21-SEP-2023   9:39:43

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

What are all of these files???

0_NORMAL_EXIT	H.ion.nc	ch4.FA
BASIS_ENTHALPY	H.ion.xml	ch4.KP
BASIS_HARRIS_ENTHALPY	H.psf	ch4.ORB_INDX
C.gga.psf	INPUT_TMP.45433	ch4.STRUCT_OUT
C.ion	MESSAGES	ch4.XV
C.ion.nc	OUTVARS.yml	ch4.alloc
C.ion.xml	PARALLEL_DIST	ch4.bib
C.psf	TIMES	ch4.contrib.EPSIMG
CLOCK	ch4.BONDS	ch4.fdf
FORCE_STRESS	ch4.BONDS_FINAL	ch4.out
H.gga.psf	ch4.DM	ch4.times
H.ion	ch4.EIG	fdf.20230921T093943.534.log

What are all of these files???

Density Matrix Restart

Forces on atoms

Coordinate Restart

```
0_NORMAL_EXIT
BASIS_ENTHALPY
BASIS_HARRIS_ENTHALPY
C.gga.psf
C.ion
C.ion.nc
C.ion.xml
C.psf
CLOCK
FORCE_STRESS
H.gga.psf
H.ion
H.ion.nc
H.ion.xml
H.psf
INPUT_TMP.45433
MESSAGES
OUTVARS.yml
PARALLEL_DIST
TIMES
ch4.BONDS
ch4.BONDS_FINAL
ch4.DM
ch4.EIG
ch4.FA
ch4.KP
ch4.ORB_INDX
ch4.STRUCT_OUT
ch4.XV
ch4.alloc
ch4.bib
ch4.contrib.EPSIMG
ch4.fdf
ch4.out
ch4.times
fdf.20230921T093943.534.log
```

Forces and Stress

KS eigenvalues

Timing information

What are all of these files???

0_NORMAL_EXIT	H.ion.nc	ch4.FA
BASIS_ENTHALPY	H.ion.xml	ch4.KP
BASIS_HARRIS_ENTHALPY	H.psf	ch4.ORB_INDX
C.gga.psf	INPUT_TMP.45433	ch4.STRUCT_OUT
C.ion	MESSAGES	ch4.XV
C.ion.nc	OUTVARS.yml	ch4.alloc
C.ion.xml	PARALLEL_DIST	ch4.bib
C.psf	TIMES	ch4.contrib.EPSIMG
CLOCK	ch4.BONDS	ch4.fdf
FORCE_STRESS	ch4.BONDS_FINAL	ch4.out
H.gga.psf	ch4.DM	ch4.times
H.ion	ch4.EIG	fdf.20230921T093943.534.log

General Output file: log, out, **you** name it

Outputs

Things we have in our FDF file

```
***** Dump of input data file *****
#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
#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
#Atomic coordinates
AtomicCoordinatesFormat Ang
%block AtomicCoordinatesAndAtomicSpecies
  0.000 0.000 0.000 1
  1.219 -0.284 -0.377 2
 -0.284 1.219 -0.377 2
 -0.140 -0.140 1.219 2
 -0.833 -0.833 -0.503 2
%endblock AtomicCoordinatesAndAtomicSpecies
# Basis set definition
PAO.EnergyShift 250 meV
PAO.SplitNorm 0.15
PAO.BasisSize SZ
#Real space grid
MeshCutoff 125.0 Ry
# Convergence of SCF
MaxSCFIterations 50
DM.MixingWeight 0.4
DM.NumberPulay 2
# Type of solution
SolutionMethod diagon
***** End of input data file *****
```

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

---- Processing specs for species: C
Ground state valence configuration: 2s02 2p02
Reading pseudopotential information in formatted form from:
  C.psf

---- Processing specs for species: H
Ground state valence configuration: 1s01
Reading pseudopotential information in formatted form from:
  H.psf

---- Pseudopotential check for C

Pseudized shells:
2s( 2.00) rc: 1.29
2p( 2.00) rc: 1.29
3d( 0.00) rc: 1.29
4f( 0.00) rc: 1.29
Valence configuration for ps generation: (assumed as above)

---- Pseudopotential check for H

Pseudized shells:
1s( 1.00) rc: 1.25
2p( 0.00) rc: 1.25
3d( 0.00) rc: 1.25
4f( 0.00) rc: 1.25
Valence configuration for ps generation: (assumed as above)
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.
For H, standard SIESTA heuristics set lmxkb to 1
(one more than the basis l, including polarization orbitals).
Use PS.lmax or PS.KBprojectors blocks to override.
```

Species and pseudopotential information

Outputs

Basis set generation (next session!)

```
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= 0.018374 Ry

  izeta = 1
          lambda = 1.000000
          rc = 4.191849
          energy = -0.983900
          kinetic = 0.912099
  potential(screened) = -1.895999
  potential(ionic) = -5.500930

SPLIT: Orbitals with angular momentum L= 1

SPLIT: Basis orbitals for state 2p

SPLIT: PAO cut-off radius determined from an
SPLIT: energy shift= 0.018374 Ry

  izeta = 1
          lambda = 1.000000
          rc = 4.993604
          energy = -0.381878
          kinetic = 2.577411
  potential(screened) = -2.959289
  potential(ionic) = -6.460511
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

Vna: Cut-off radius for the neutral-atom potential: 4.993604
```

Outputs

Coordinates and selected options

```

coord: Atomic-coordinates input format = Cartesian coordinates
coord: (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      25

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 Pop. = NO
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
redata: Mix DM in first SCF step = T
redata: Write Pulay info on disk = 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...
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 overlapping 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
```

Type of run, cell information.

Sparsity information.

Mesh information (tomorrow!)

Outputs

```
siesta: Program's energy decomposition (eV):  
siesta: Ebs      =      -86.773862  
siesta: Eions    =      383.324493  
siesta: Ena      =      115.426770  
siesta: Ekin     =      143.738590  
siesta: Enl      =     -16.728728  
siesta: Eso      =       0.000000  
siesta: Edftu    =       0.000000  
siesta: DEna     =       1.592579  
siesta: DUscaf   =       0.349516  
siesta: DUext    =       0.000000  
siesta: Ex       =     -64.874822  
siesta: Ec       =     -10.703118  
siesta: Exc      =     -75.577940  
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  =    -223.671697  
siesta: Etot     =    -214.523706  
siesta: FreeEng  =    -214.523706
```

Initial, non-SCF energy
decomposition.

Outputs

```
      iscf      Eharris(eV)      E_KS(eV)      FreeEng(eV)      dDmax      Ef(eV) dHmax(eV)
scf:    1      -223.671697      -214.523706      -214.523706      1.090911      -7.083002      1.436999
timer: Routine,Calls,Time,% = IterSCF      1      0.133 29.48
scf:    2      -214.585551      -214.573147      -214.573147      0.040577      -6.647325      0.203018
scf:    3      -214.573456      -214.573477      -214.573477      0.004139      -6.585363      0.150120
scf:    4      -214.573442      -214.573493      -214.573493      0.002062      -6.424159      0.074339
scf:    5      -214.573514      -214.573506      -214.573506      0.000928      -6.476298      0.003034
scf:    6      -214.573506      -214.573506      -214.573506      0.000039      -6.474131      0.000389
```

SCF Convergence by DM+H criterion

max |DM_out - DM_in| : 0.0000385344

max |H_out - H_in| (eV) : 0.0003888059

SCF cycle converged after 6 iterations

Using DM_out to compute the final energy and forces

No. of atoms with KB's overlapping orbs in proc 0. Max # of overlaps: 5 8

siesta: E_KS(eV) = -214.5735

siesta: E_KS - E_eggbbox = -214.5735

siesta: Atomic forces (eV/Ang):

Tot 0.000066 0.000066 -0.001085

Max 2.352006
Res 1.126956 sqrt(Sum f_i^2 / 3N)

Max 2.352006 constrained

Stress tensor Voigt[x,y,z,yz,xz,xy] (kbar): 1.99 1.99 0.95 -0.20

(Free)E + p*V (eV/cell) -218.0329

Target enthalpy (eV/cell) -214.5735

SCF cycle information

Converged KS energy

Converged total forces and
cell stress

Final energy decomposition

```
siesta: Program's energy decomposition (eV):
siesta: Ebs      =      -90.137390
siesta: Eions    =      383.324493
siesta: Ena      =      115.426770
siesta: Ekin     =      141.310823
siesta: Enl      =     -16.669337
siesta: Eso      =       0.000000
siesta: Edftu    =       0.000000
siesta: DEna     =       3.517376
siesta: DUskf    =       0.257037
siesta: DUext    =       0.000000
siesta: Ex       =     -64.416938
siesta: Ec       =     -10.674744
siesta: Exc      =     -75.091682
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  =     -214.573506
siesta: Etot     =     -214.573506
siesta: FreeEng  =     -214.573506

siesta: Final energy (eV):
siesta: Band Struct. =     -90.137390
siesta: Kinetic      =      141.310823
siesta: Hartree      =      282.193258
siesta: Edftu        =       0.000000
siesta: Eso          =       0.000000
siesta: Ext. field   =       0.000000
siesta: Exch.        =     -64.416938
siesta: Corr.        =     -10.674744
siesta: Bulk bias    =       0.000000
siesta: Exch.-corr.  =     -75.091682
siesta: Ion-electron =     -697.792327
siesta: Ion-ion      =      134.806422
siesta: Ekinion      =       0.000000
siesta: D3 dispersion =       0.000000
siesta: Total        =     -214.573506
siesta: Fermi        =     -6.474131
```

Final forces

Final stress/pressure

Electric dipole

```
siesta: Atomic forces (eV/Ang):
siesta:      1      0.152980      0.152980     -1.053682
siesta:      2     -2.352006      0.483512      0.761553
siesta:      3      0.483512     -2.352006      0.761553
siesta:      4      0.342189      0.342189     -0.971719
siesta:      5      1.373392      1.373392      0.501211
siesta: -----
siesta:      Tot      0.000066      0.000066     -0.001085

siesta: Stress tensor (static) (eV/Ang**3):
siesta:      0.001241     -0.000019     -0.000128
siesta:     -0.000019      0.001241     -0.000128
siesta:     -0.000128     -0.000128      0.000593

siesta: Cell volume =          3375.000000 Ang**3

siesta: Pressure (static):
siesta:      Solid              Molecule  Units
siesta:     -0.00001116          0.00000003 Ry/Bohr**3
siesta:     -0.00102500          0.00000251 eV/Ang**3
siesta:     -1.64224685          0.00402704 kBar
(Free)E+ p_basis*V_orbitals =          -214.071102
(Free)Eharris+ p_basis*V_orbitals =          -214.071102

siesta: Electric dipole (a.u.) =     -0.011992     -0.011992      0.008053
siesta: Electric dipole (Debye) =     -0.030480     -0.030480      0.020469
```

Primary bibliography, and end-of-run time

```
cite: Please see "ch4.bib" for an exhaustive BiBTeX file.  
cite: Please clearly indicate Siesta version in published work:  
cite: This calculation has made use of the following articles  
cite: which are encouraged to be cited in a published work.  
      Primary SIESTA paper  
      DOI: www.doi.org/10.1088/0953-8984/14/11/302  
  
>> End of run: 21-SEP-2023 9:39:44  
Job| completed
```


What else is there?

A look at the SIESTA suite:

Eig2DOS	dm_creator	fmpdos	grid_supercell	mprop	plsts	siesta	vib2xsf
cdf2dm	dm_noncol_sign_flip4	fractional	horizontal	ol-stm	protoNEB	simplex	vibra
cdf2grid	dmbs2dm	g2c_ng	hs2hsx	optical	psml2psf	sockets_parallel	wfs2wfsx
cdf2xsf	dmfilter	gen-basis	hsx2hs	optical_input	psop	sockets_serial	wfsnc2wfsx
cdf_diff	eig2bxsf	getResults	ioncat	orbmol_proj	pvtsp	spin_texture	wfsx2wfs
cdf_fft	eigfat2plot	gnubands	ionplot.sh	pdosxml	read_spin_texture	swarm	xv2xsf
cdf_get_cell	f2fmaster	grid1d	lwf2cdf	permute	readwf	tbtrans	
cdf_laplacian	f2fslave	grid2cdf	macroave	phonons	readwfx	ts2ts	
countJobs	fat	grid2cube	mctc-convert	phtrans	rho2xsf	tscontour	
denchar	fcbuild	grid2d	md2axsf	pipes_parallel	runJobs	tshs2tshs	
dm2cdf	fdf2grimme	grid2val	mixps	pipes_serial	s-dftd3	unfold	
dmUnblock	fmixmd-driver	grid_rotate	mpi_driver	plstm	sies2arc	v_info	

Utilities and others

A look at the SIESTA suite:

Eig2DOS	dm_creator	fmpdos	grid_supercell	mprop	plsts	siesta	vib2xsf
cdf2dm	dm_noncol_sign_flip4	fractional	horizontal	ol-stm	protoNEB	simplex	vibra
cdf2grid	dmbs2dm	g2c_ng	hs2hsx	optical	psml2psf	sockets_parallel	wfs2wfsx
cdf2xsf	dmfilter	gen-basis	hsx2hs	optical_input	psop	sockets_serial	wfsnc2wfsx
cdf_diff	eig2bxsf	getResults	ioncat	orbmol_proj	pvtsp	spin_texture	wfsx2wfs
cdf_fft	eigfat2plot	gnubands	ionplot.sh	pdosxml	read_spin_texture	swarm	xv2xsf
cdf_get_cell	f2fmaster	grid1d	lwf2cdf	permute	readwf	tbtrans	
cdf_laplacian	f2fslave	grid2cdf	macroave	phonons	readwfx	ts2ts	
countJobs	fat	grid2cube	mctc-convert	phtrans	rho2xsf	tscontour	
denchar	fcbuild	grid2d	md2axsf	pipes_parallel	runJobs	ts2ts	
dm2cdf	fdf2grimme	grid2val	mixps	pipes_serial	s-dftd3	unfold	
dmUnblock	fmixmd-driver	grid_rotate	mpi_driver	plstm	sies2arc	v_info	

Utilities and others

Some utilities we will use later...

Eig2DOS	dm_creator	fmpdos	grid_supercell	mprop	plsts	siesta	vibron
fat	dm_noncol_sign_flip4	fractional	horizontal	plot	protoNEB	simplex	vibra
cdf2grid	dmbs2dm	g2c_ng	hs2hsx	optical	psml2psf	sockets_parallel	wfsnc2wfsx
cdf2xsf	dmfilter	gen-basis	hsx2hs	optical_input	psop	sockets_serial	wfsx2wfs
cdf_diff	eig2bxsf	getResults	ioncat	orbmol_proj	pvtsp	spin_texture	xv2xsf
cdf_fft	eigfat2plot	gnubands	ionplot.sh	pdosxml	read_spin_texture	swarm	
cdf_get_cell	f2fmaster	grid1d	lwf2cdf	permute	readwf	tbtrans	
cdf_laplacian	fat2cube	grid2cdf	macroave	phonons	readwfx	ts2ts	
denchar	fat	grid2cube	mctc-convert	phtrans	rho2xsf	tscontour	
dmUnblock	fat2plot	grid2d	md2axsf	pipes_parallel	runJobs	tshs2tshs	
	fdf2grimme	grid2val	mixps	pipes_serial	s-dftd3	unfold	
	fmixmd-driver	grid_rotate	mpi_driver	plstm	sies2arc	v_info	

Format converters to help with visualization


Eig2DOS	dm_creator	fmpdos	grid_supercell	mprop	plsts	siesta	vib2xsf
cdf2dm	dm_noncol_sign_flip4	g2c_ng	horizontal	ol-stm	protoNEB	simplex	wfs2wfsx
cdf2grid	dmbs2dm	gnubands	hs2hsx	optical	psml2psf	sockets_parallel	wfsnc2wfsx
cdf2xsf	dmfilter	grid2cube	hsx2hs	optical_input	psop	sockets_serial	xv2xsf
cdf_diff	eig2bxsf	ionplot.sh	ionplot	orbmol_proj	pvtsp	spin_texture	
cdf_fft	eigfat2plot	macroave	md2axsf	pdosxml	read_spin_texture	swarm	
cdf_get_cell	f2fmaster	grid2val	mpi_driver	permute	readwf	tbtrans	
cdf_laplacian	f2fslave	grid_rotate		phonons	rho2xsf	ts2ts	
countJobs	fat			phtrans	s-dftd3	tscontour	
denchar	fcbuild			pipes_parallel	sies2arc	ts2ts	
dm2cdf	fdf2grimme			pipes_serial		tscontour	
dmUnblock	fmixmd-driver			plstm		ts2ts	

Choosing a pseudo

Choosing a pseudo

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

[Help me](#)



PSEUDO DŌJŌ

[Download](#)

Mean

3.13

hints tests

32.74 0.95

37.25 2.20

43.36 -0.09

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Select the flavor and [format](#), then click "Download" to get the complete table of pseudos or choose a specific element. "HTML" gives full test results.

Type	XC	Accuracy	Format
NC SR (ONCVPSP v0.5)	PBE	standard	psp8

1 H 1	2 He 2	3 Li 3	4 Be 2	5 B 2	6 C 2	7 N 2	8 O 2	9 F 2	10 Ne 2
11 Na 3	12 Mg 3	13 Al 3	14 Si 2	15 P 2	16 S 2	17 Cl 2	18 Ar 2	19 K 3	20 Ca 3
21 Sc 4	22 Ti 4	23 V 4	24 Cr 4	25 Mn 4	26 Fe 4	27 Co 4	28 Ni 4	29 Cu 4	30 Zn 4
31 Ga 3	32 Ge 3	33 As 3	34 Se 3	35 Br 3	36 Kr 3	37 Rb 3	38 Sr 3	39 Y 3	40 Zr 3
41 Nb 3	42 Mo 3	43 Tc 3	44 Ru 3	45 Rh 3	46 Pd 3	47 Ag 3	48 Cd 3	49 In 3	50 Sn 3
51 Sb 3	52 Te 3	53 I 3	54 Xe 3	55 Cs 3	56 Ba 3	57 La 3	58 Ce 3	59 Pr 3	60 Nd 3
61 Pm 3	62 Sm 3	63 Eu 3	64 Gd 3	65 Tb 3	66 Dy 3	67 Ho 3	68 Er 3	69 Tm 3	70 Yb 3
71 Lu 3	72 Hf 3	73 Ta 3	74 W 3	75 Re 3	76 Os 3	77 Ir 3	78 Pt 3	79 Au 3	80 Hg 3
81 Tl 3	82 Pb 3	83 Bi 3	84 Po 3	85 At 3	86 Rn 3	87 Fr 3	88 Ra 3	89 Ac 3	90 Th 3
91 Pa 3	92 U 3	93 Np 3	94 Pu 3	95 Am 3	96 Cm 3	97 Bk 3	98 Cf 3	99 Es 3	100 Fm 3
101 Md 3	102 No 3	103 Lr 3	104 Rf 3	105 Db 3	106 Sg 3	107 Bh 3	108 Hs 3	109 Mt 3	110 Ds 3
111 Rg 3	112 Cn 3	113 Nh 3	114 Fl 3	115 Mc 3	116 Lv 3	117 Ts 3	118 Og 3	119 Uu 3	120 Uub 3
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Choosing a pseudo

- If you want more control, you can generate your own pseudopotentials using ATOM (<https://docs.siesta-project.org/projects/atom/en/latest/tutorial/ps-generation/index.html>)
- Remember to always *read the literature* carefully and *test your pseudos* accordingly.

Choosing functional

Choosing a DFT functional

SIESTA offers different families of DFT functionals:

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

Choosing a DFT functional

In the tutorials for **day1** go to **02-LevelOfTheory**, remember to copy the run script from `/gpfs/projects/nct_315/SCRIPTS/runmn.sh`.

Follow the steps in the DFT Functional section of:

<https://docs.siesta-project.org/projects/siesta/en/latest/tutorials/basic/first-encounter-theorylevel/index.html>

A First Encounter - Part 2: Choosing your level of theory

Choosing a Pseudopotential

An important thing that determines the quality of the calculation is the choice of the pseudopotential. As mentioned in [A First Encounter - Part 1: Running SIESTA](#), pseudopotentials in SIESTA are provided as external input files, usually in psf or psml formats.

Generating a new pseudopotential from scratch is outside the scope of this tutorial, but more information can be seen in [Pseudopotentials](#). For most cases, you can instead download pre-

Have you set up the local environment?

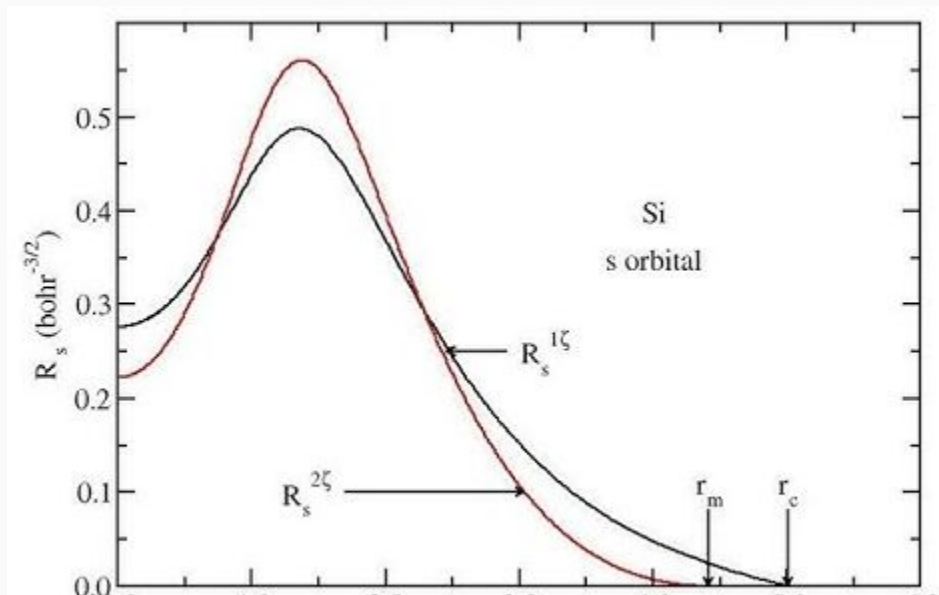
If not, [do that now](#) before proceeding.

A peek into basis sets

A peek into basis sets

SIESTA's basis sets are at the core of its efficiency.

For now, suffice to say that SIESTA has atomic-centered basis functions, that become zero after a certain cut-off radius.



A peek into basis sets

For now, we will only concern ourselves with:

- Exploring the basis set cardinality (SZ, SZP, DZP), 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.

We will cover this more in-depth in the upcoming sessions!

First tests with water (geometry optimization)

Follow the steps in the **Playing with CH4** section of:

<https://docs.siesta-project.org/projects/siesta/en/latest/tutorials/basic/first-encounter-theorylevel/index.html>

Take note of how the **total energy (from output)**, **bond lengths (ch4.BONDS_FINAL file)**, and **total time (from ch4.times)** change in these cases:

- 1) When changing the basis set between **SZ, SZP, and DZP**. Use an energy shift of **250 meV**.

```
PAO.BasisSize    DZP
```

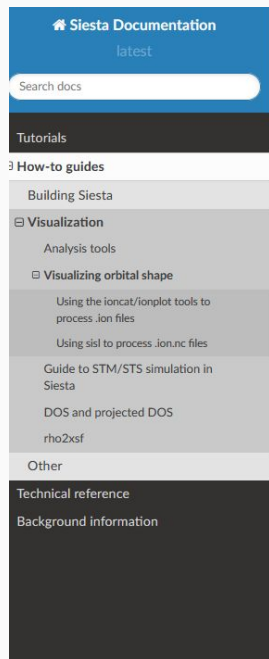
- 2) For **DZP**, changing the energy shift between **5 meV, 100 meV, and 500 meV**.

```
PAO.EnergyShift  0.01 Ry
```

TIP: Visualizing orbital shapes

How-to -> Visualization -> Visualizing Orbital Shapes

<https://docs.siesta-project.org/projects/siesta/en/latest/how-to/visualization/orbitals.html>



» How-to guides » Visualizing orbital shape

[Edit on GitLab](#)

Visualizing orbital shape

Using the ioncat/ionplot tools to process .ion files

You can look at the shape of the orbitals by plotting the contents of the .ion files produced by Siesta. These files are not easily readable, but the 'ioncat' program can extract the relevant pieces of information, and the "ionplot" script can drive 'ioncat' to plot the desired graphs. For example:

```
ionplot -o 1 0
```

will plot the orbital with number "1" in the O.ion file.:

```
ioncat -i 0
```

will print the numbers of the representative orbitals of each nlz shell (i.e., disregarding the 'm' quantum number, which does not affect the radial part).:

```
ioncat -o 1 0
```

will output the data for the first orbital in O.ion.

Typing `ioncat -h` produces a display of the full set of options for the program:

Questions?