A first encounter with siesta™

11/11/2024 - Federico Pedron

ICN2 Institut Català de Nanociència i Nanotecnologia
Barcelona Supercomputing Center
Centro Nacional de Supercomputación
CSIC Consejo Superior de Investigaciones Científicas

MAX DRIVING THE EXASCALE TRANSITION
Ministerio de Ciencia, Innovación y Universidades
Financiado por la Unión Europea NextGenerationEU
Plan de Recuperación, Transformación y Resiliencia
Agencia Estatal de Investigación

How do we run siesta™?

Reminder: how to connect

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

Reminder: how to connect

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 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

#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

#Real space grid
MeshCutoff 125.0 Ry

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

# Type of solution
SolutionMethod diagon
```

Basis Set Options

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

Options for SCF acceleration.

Solver options.

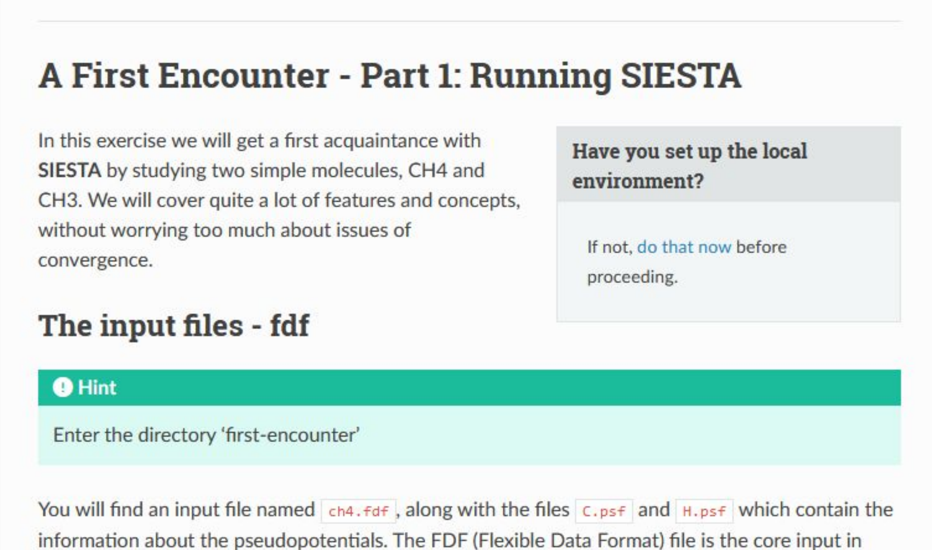
Let’s try it!

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…

Outputs

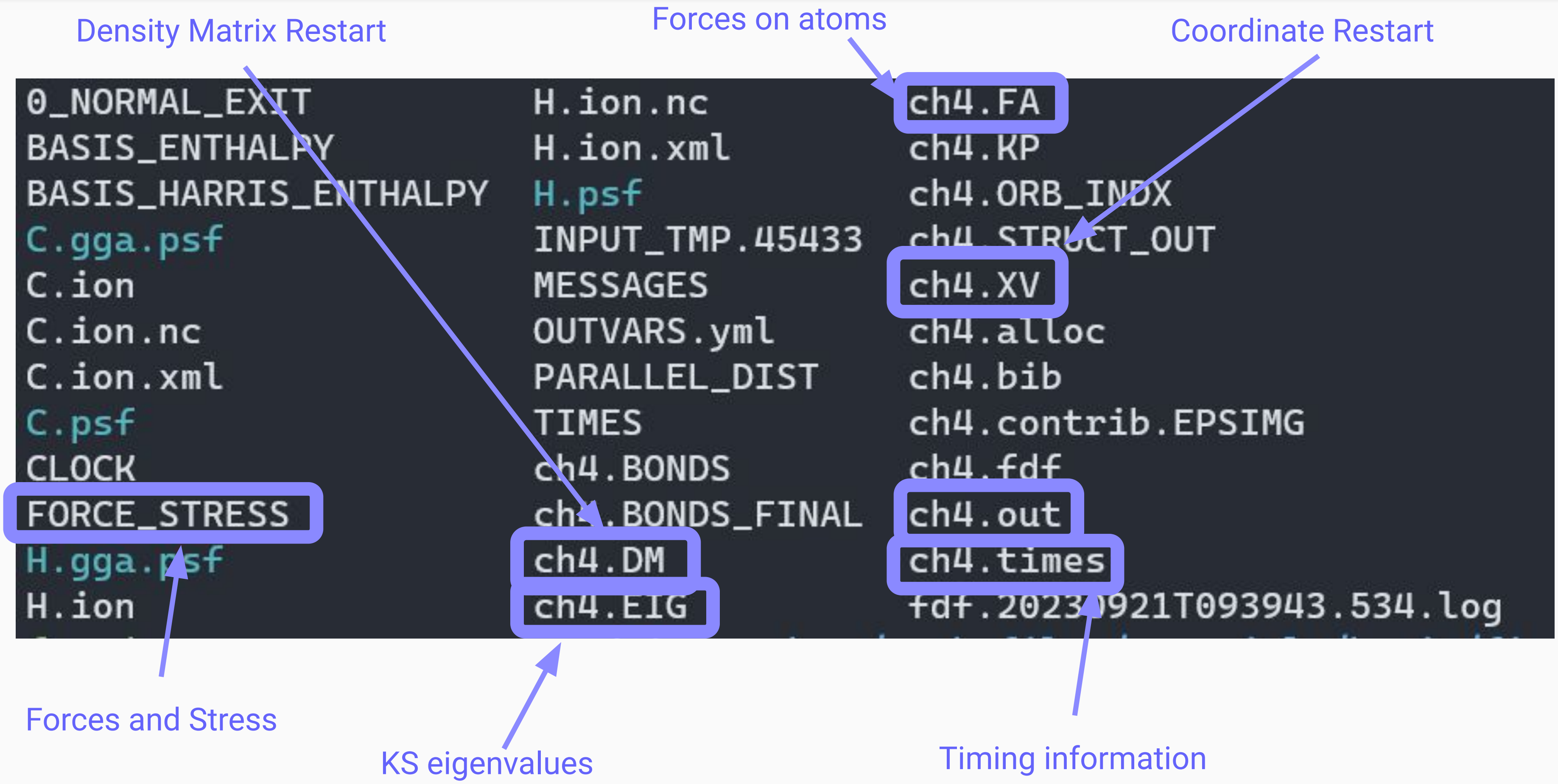
Installation and run info, Start Time

```
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???



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

```
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
```

Basis set generation (next session!)

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    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 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
```

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: DUscf   =         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 overlaping orbs in proc 0. Max # of overlaps:       5       8

siesta: E_KS(eV) =             -214.5735

siesta: E_KS - E_eggbox =      -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

Outputs

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: DUscf   =         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
```

Outputs

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
```

Outputs

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?

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              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                                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

Some utilities we will use later…

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

Utilities and others

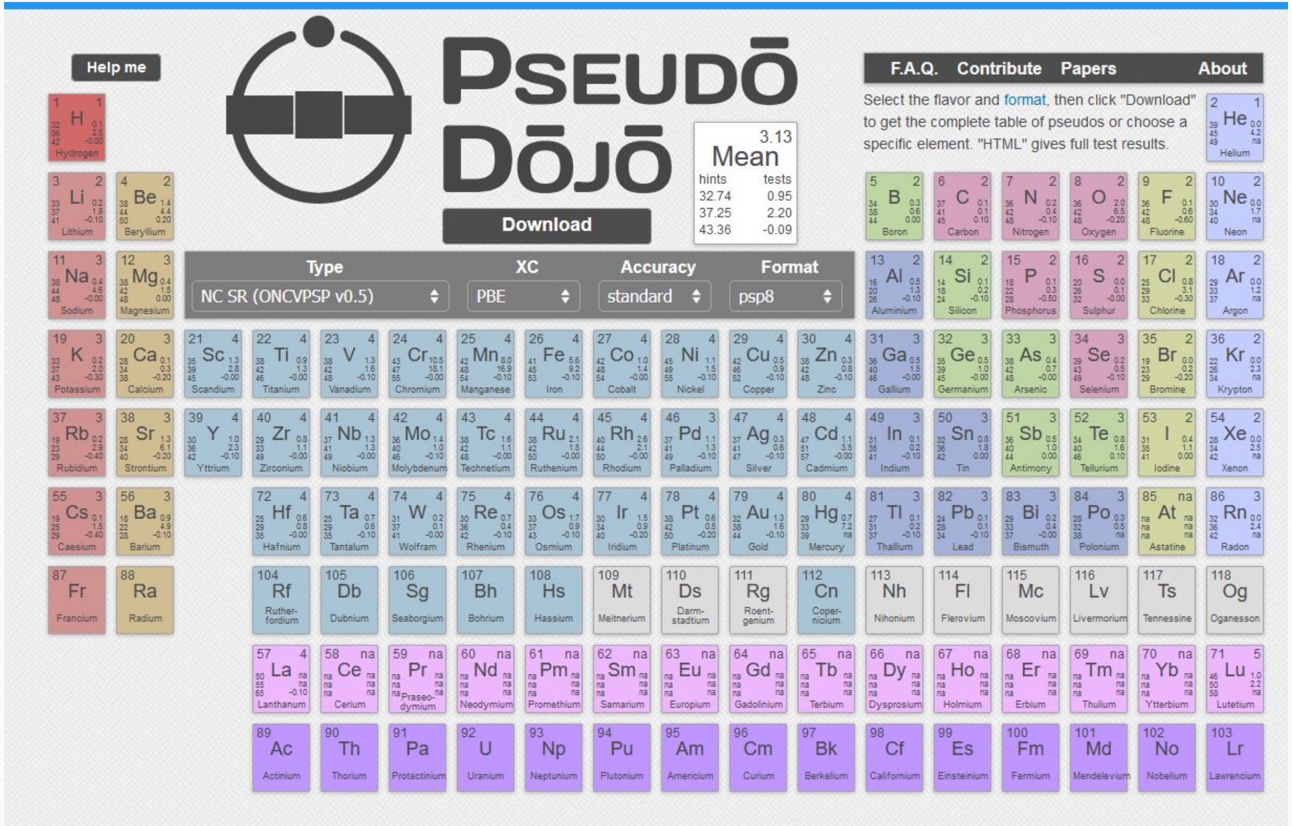
Format converters to help with visualization

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

Choosing a pseudo

Choosing a pseudo

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



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.

Have you set up the local environment?

If not, do that now before proceeding.

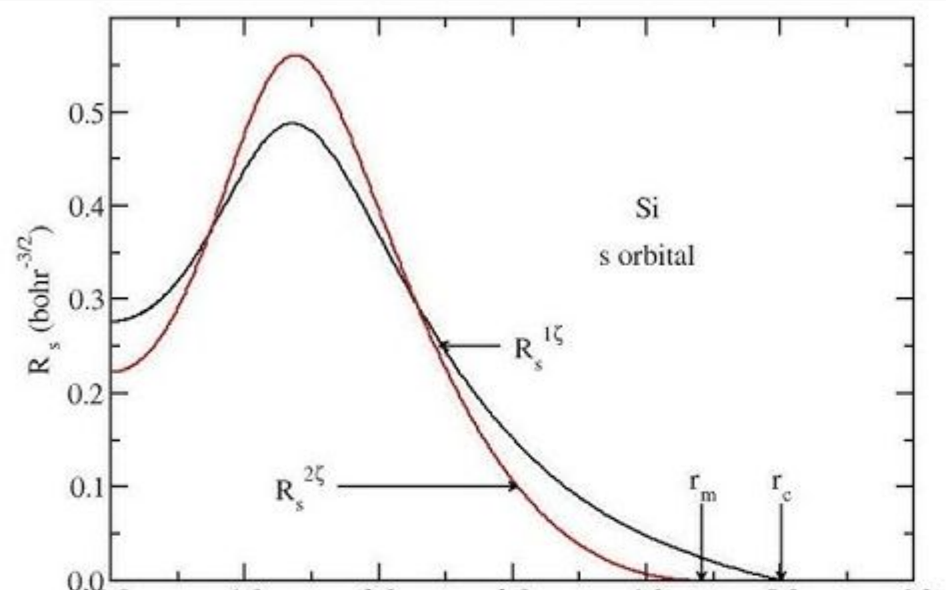
Generating a new pseudopotential from scratch is outside the scope of this tutorial, but more information can be seen in Pseudopotentials. For most cases, you can instead download pre-

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
```

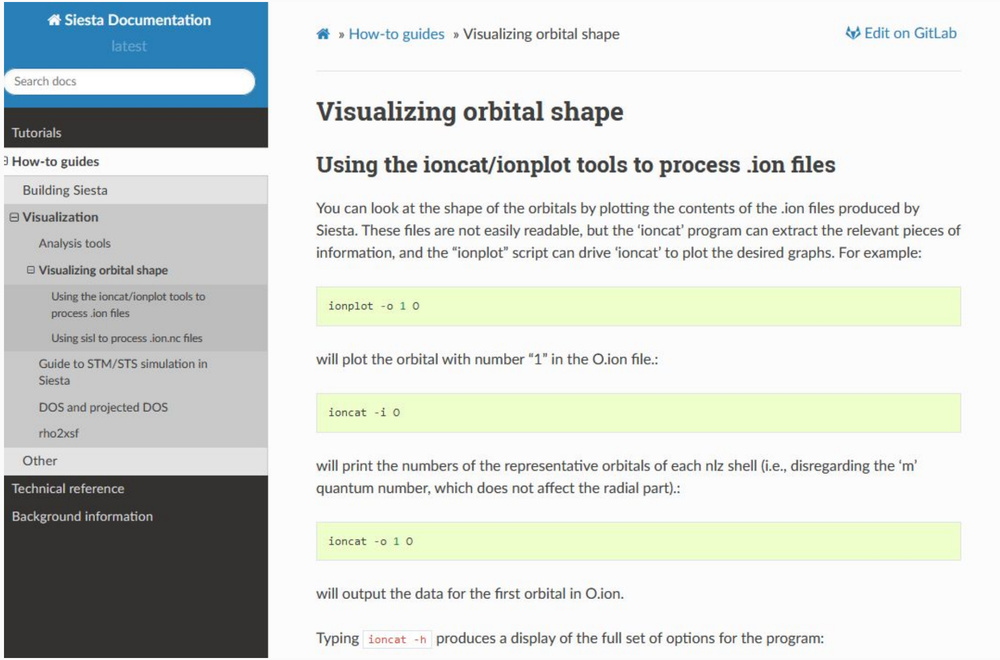
2) For **DZP**, changing the energy shift between **5 meV, 100 meV, and 500 meV**.

```
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



Questions?