A first encounter with siesta™

02/10/2023 - Federico Pedron

How do we run siesta?

™

Reminder: how to connect

https://siesta-project.org/siesta/events/SIESTA_School-2023/MN4.html

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SIESTA School 2023: MareNostrum 4

MareNostrum 4 is the largest operational supercomputer of the Barcelona Supercomputing Center. Each node contains 2 Intel Xeon Platinum processors (with 24 cores each) and 96 GB of RAM. They all run SUSE Linux 12.

You should have received your BSC credentials in your institutional email account on September 30th. Your BSC account is already enabled. Please contact the organisers if you have not received this email.

Connecting to MN4

From your computer terminal, use your SSH client to connect to a MN4 login node. There are three login nodes, `mn1.bsc.es`, `mn2.bsc.es`, and `mn3.bsc.es`. You can connect to any of them, they are used interchangeably in the examples below.

Via conventional SSH client (Mac, Linux, Windows with WSL/Cygwin)

From a terminal, run

```
$ ssh <USERNAME>@mn1.bsc.es
```

where `<USERNAME>` is your BSC username (e.g., `ctn99999`). You will be prompted for the corresponding password.

If you want to enable visualization, you need to use the `-X` option:

```
$ ssh -X <USERNAME>@mn1.bsc.es
```

Via PuTTY or mobaXterm

If you don't have any SSH client installed in your computer, please download and install mobaXterm (recommended) or PuTTY.

When you open the graphical interface define the server/host name (`mn3.bsc.es`) and provide your username and password when prompted. For mobaXterm, there is a short generic demo video available here.

For visualizations using PuTTY, please keep in mind the following:

- Under connection → SSH → X11, make sure that the "Enable X11 forwarding" option is checked.
- You also need to install xMing.

In mobaXterm this is enabled by default.

Reminder: how to connect

https://siesta-project.org/siesta/events/SIESTA_School-2023/MN4.html

ssh nct01YYY@mn1.bsc.es

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

Use also mn2, mn3! (only for data/password: dt01.bsc.es)

Then:

cd /gpfs/scratch/nct01/nct01YYY (we will run things here)

Reminder: tutorial files

Each day, you should copy the tutorial folder available at

/gpfs/projects/nct00/nct00003/TUTORIALS/dayX

For example:

```
cp -r /gpfs/projects/nct00/nct00003/TUTORIALS/day1  day1
```

Submitting a job

In each run folder, copy the sample run script from
/gpfs/projects/nct00/nct00003/SCRIPTS/runmn.sh

```
cp  /gpfs/projects/nct00/nct00003/SCRIPTS/runmn.sh 1-FirstEncounter/CH4/.
cp  /gpfs/projects/nct00/nct00003/SCRIPTS/runmn.sh 1-FirstEncounter/CH3/.
```

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 -D .

# DO NOT CHANGE THIS LINE
source /gpfs/projects/nct00/nct00003/siestarc.sh

# EDIT 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 -D .

# DO NOT CHANGE THIS LINE
source /gpfs/projects/nct00/nct00003/siestarc.sh

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

Submitting a job

Submit!

sbatch runmn.sh

To use reservations:

sbatch runmn.sh --reservation=SIESTA-DAY

sbatch runmn.sh --reservation=SIESTA-NIGHT

https://siesta-project.org/siesta/events/SIESTA_School-2023/MN4.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 (last part is optional)

1) ssh nct01YYY@mn2.bsc.es ← (also mn1, mn3)
2) cd /gpfs/scratch/nct01/nct01YYY
3) cp /gpfs/projects/nct00/nct00003/TUTORIALS/day1 .
4) cp /gpfs/projects/nct00/nct00003/SCRIPTS/runmn.sh .
5) (move and edit runmn.sh to your run folders)
6) sbatch runmn.sh

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???

Density Matrix Restart

Forces on atoms

Coordinate Restart

```
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
```

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

```
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
```