Basic introduction to running Siesta

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Our method

Linear-scaling DFT based on
NAOs (Numerical Atomic Orbitals)

P. Ordejon, E. Artacho & J. M. Soler , Phys. Rev. B 53, R10441 (1996)

J. M.Soler et al, J. Phys.: Condens. Matter **14**, 2745 (2002)

- •Born-Oppenheimer (relaxations, mol.dynamics)
- •DFT (LDA, GGA)
- •Pseudopotentials (norm conserving,factorised)
- •Numerical atomic orbitals as basis (finite range)
- •Numerical evaluation of matrix elements (3Dgrid)

Implemented in the SIESTA **method:**

D. Sanchez-Portal, P. Ordejon, E. Artacho & J. M. Soler
Int. J. Quantum Chem. 65, 453 (1997)

Siesta resources (I)

- Web page: http://www.uam.es/siesta
- Pseudos and basis database
- Mailing list
- Usage manual
- Soon: http://cygni.fmc.uam.es/mediawiki
- Issue tracker (for bugs, etc)
- Mailing list archives
- Wiki

Siesta resources (2)

- Andrei Postnikov Siesta utils page:

  http://www.home.uni-osnabrueck.de/apostnik/download.html

- Lev Kantorovich Siesta utils page:

  http://www.cmmp.ucl.ac.uk/~lev/codes/lev00/index.html

Siesta software package:

- Src: Sources of the Siesta code.
- Src/Sys: makefiles for the compilation
- Src/Tests: A collection of tests.
- Docs: Documentation and user conditions:
  - User's Guide (siesta.tex)
- Pseudo: ATOM program to generate and test pseudos.

(A. García; *Pseudopotential and basis generation*, Tu 11:10)

- Examples: fdf and pseudos input files for simple systems.
- Tutorials: Tutorials for basis and pseudo generation.
- Utils: Programs or scripts to analyze the results.

To run Siesta you need:

1.- Access to the executable file: T. White: "***And now that you are back at home ... what?***" Friday 13:00.

2.- An input file: written in ascii (plain text) using:

Flexible Data Format (FDF) (A. García and J. M. Soler)

3.- A pseudopotential file for each kind of element in the input file. Two different formats:

Unformatted binary (.vps)

Formatted ASCII (.psf) (more transportable and easy to look at)

Running siesta

Siesta has no windows, it is run from a UNIX terminal or from a MSDOS console.

Main input file: “name”.fdf

•Contents:

•Physical data of the system

•Variables to control the aproximations

•Format:

•Flexible Data Format (FDF) developed by A. García and J. M. Soler

FDF (I)

•Data can be given in any order

•Data can be omitted in favor of default values

•Syntax: ‘data label’ followed by its value

Character string:	SystemLabel	h2o
Integer:	NumberOfAtoms	3
Real:	PAO.SplitNorm	0.15
Logical:	SpinPolarized	.false.
Physical magnitudes	LatticeConstant	5.43 Ang

FDF (II)

• Labels are case insensitive and characters -_. are ignored

LatticeConstant is equivalent to lattice_constant

• Text following # are comments

• Logical values: T , .true. , yes, F , .false. , no

By default logicals are true: DM.UseSaveDM

• Character strings, NOT in apostrophes

• Complex data structures: blocks

```
%block label
…
%endblock label
```

FDF (III)

• Physical magnitudes: followed by its units.

Many physical units are recognized for each magnitude

(Length: m, cm, nm, Ang, bohr)

Automatic conversion to the ones internally required.

• You may 'include' other FDF files or redirect the search to another file, so for example in the main fdf it's possible:

```
AtomicCoordinatesFormat < system_xyz.fdf

AtomicCoordinatesAndAtomicSpecies  < system_xyz.fdf
```

Basic input variables

1.- General system descriptors

2.- Structural and geometrical variables

3.- Functional and solution mehod (Order-N/diagonalization)

4.- Convergence of the results

5.- Self-consistency

6.- Basis set generation related variables:

“*How to test and generate basis sets*”, Tu 12:00

General system descriptor: output

SystemName: descriptive name of the system

```
SystemName   Si bulk, diamond structure
```

SystemLabel: nickname of the system to name output files

```
SystemLabel   Si
```

(After a successful run, you should have files like

Si.DM : Density matrix

Si.XV: Final positions and velocities

...)

Structural and geometrical variables

NumberOfAtoms: number of atoms in the simulation

```
NumberOfAtoms     2
```

NumberOfSpecies: number of different atomic species

```
NumberOfSpecies   1
```

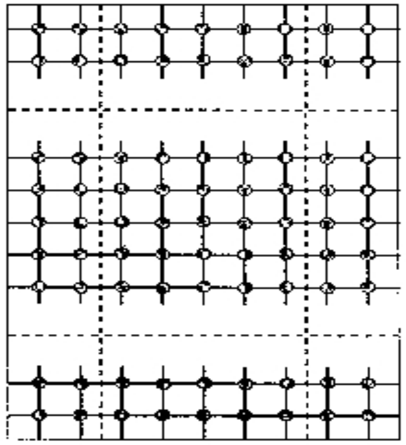
ChemicalSpeciesLabel: specify the different chemical species.

```
%block ChemicalSpeciesLabel
1      14     Si
%endblock ChemicalSpeciesLabel
```

ALL THESE VARIABLES ARE MANDATORY

Lattice Vectors

Surfaces



Atoms in the unit cell **always** are **periodically repeated throughout space** along the lattice vectors

LatticeConstant: real length to define the scale of the lattice vectors

```
LatticeConstant       5.43 Ang
```

LatticeParameters: Crystallograhic way

```
%block LatticeParameters
    1.0  1.0  1.0  60.  60.  60.
%endblock LatticeParameters
```

LatticeVectors: read as a matrix, each vector on it's own line

```
%block LatticeVectors
     0.0    0.5    0.5
     0.5    0.0    0.5
     0.5    0.5    0.0
%endblock LatticeVectors
```

Atomic Coordinates

AtomicCoordinatesFormat: format of the atomic positions in input:

Bohr: cartesian coordinates, in bohrs

Ang: cartesian coordinates, in Angstroms

ScaledCartesian: cartesian coordinates scaled to the lattice constant

Fractional: referred to the lattice vectors

```
AtomicCoordinatesFormat     Fractional
```

AtomicCoordinatesAndAtomicSpecies:

```
%block AtomicCoordinatesAndAtomicSpecies
0.00   0.00   0.00   1
0.25   0.25   0.25   1
%endblock AtomicCoordinatesAndAtomicSpecies
```

Functional

$$\begin{tikzcd}
 & & \text{DFT} \arrow[dl] \arrow[dr] & & \\
\text{XC.Functional} & \text{LDA} \arrow[d] \arrow[dr] & & \text{GGA} & \text{SpinPolarized} \\
\text{XC.authors} & \text{CA} & \text{PW92} & \text{PBE} & \\
 & \text{PZ} & & &
\end{tikzcd}$$

DFT ≡ Density Functional Theory

LDA ≡ Local Density Approximation

GGA ≡ Generalized Gradient Approximation

CA ≡ Ceperley-Alder

PZ ≡ Perdew-Zunger

PW92 ≡ Perdew-Wang-92

PBE ≡ Perdew-Burke-Ernzerhof

....

Solution method

0: Start from the atomic coordinates and the unit cell

$$\begin{tikzcd} \{\vec{R}\}_N \ \{\vec{a}\} \arrow[d] \\ \text{Hamiltonian } (H)\text{, Overlap } (S) \text{ matrices} \end{tikzcd}$$

1: Compute H,S (Order *N*):

$$\begin{tikzcd} & (H - \varepsilon S)C = 0 \arrow[dl] \arrow[dr] & \\ \text{diagon} & & \text{Order-N} \end{tikzcd}$$

2: SolutionMethod

Execution time

P. Ordejón, "*How to run with linear-scaling solvers*", Wed 11:10

k-sampling

Many magnitudes require integration of Bloch functions over Brillouin zone (BZ)

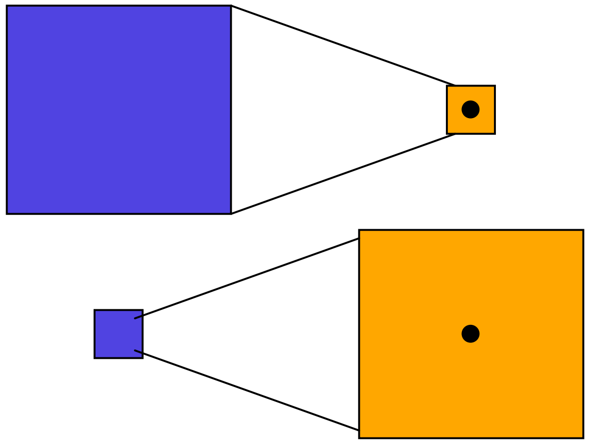
$$\rho(\vec{r}) = \sum_i \int_{BZ} d\vec{k}\, n(\vec{k}) \left|\psi_i(\vec{k})\right|^2$$

In practice: integral $\longrightarrow$ sum over a finite uniform grid

Essential for:

Small periodic systems

Real space $\leftrightarrow$ Reciprocal space



Metals

Good description of the Bloch states at the Fermi level

Magnetic systems

Even in same insulators:

Perovskite oxides

k-sampling

Special set of k-points: **Accurate results** for a **small #** k-points:

kgrid_cutoff (1): kgrid_cutoff 10.0 Ang

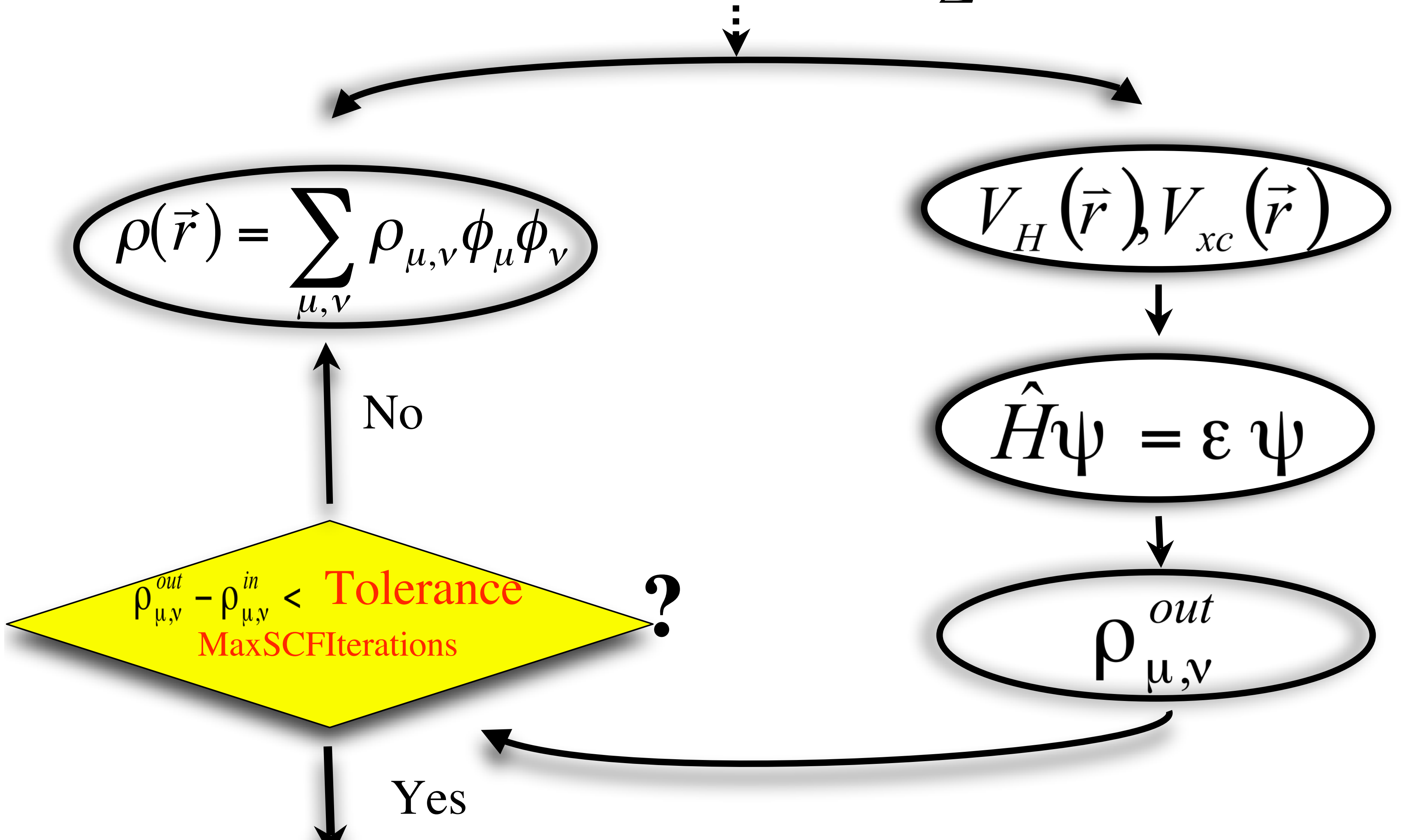
kgrid_Monkhorst_Pack (2):

```
%block kgrid_Monkhorst_Pack
    4   0   0  0.5
    0   4   0  0.5
    0   0   4  0.5
%endblock kgrid_Monkhorst_Pack
```

1 Moreno and Soler, PRB 45, 13891 (1992).
2 Monkhorst and Pack, PRB 13, 5188 (1997)

Selfconsistency (SCF)

Initial guess: $\rho(\vec{r}) = \sum \rho^{atom}(\vec{r})$


$\rho(\vec{r}) = \sum_{\mu,\nu} \rho_{\mu,\nu}\phi_\mu\phi_\nu$
$V_H(\vec{r}), V_{xc}(\vec{r})$
$\hat{H}\psi = \varepsilon\,\psi$
$\rho^{out}_{\mu,\nu}$
$\rho^{out}_{\mu,\nu} - \rho^{in}_{\mu,\nu} <$ Tolerance
MaxSCFIterations
?
No
Yes

Properties: Total energy, Charge density   Forces

How to run Siesta

To run the serial version, from a unix/terminal:

Is siesta in your PATH?
Two options:

1) Set your PATH: *export PATH=$PATH:/wherever_siesta_is*
2) Include the full path of siesta: */home/edu/siesta-2.0.1/bin/siesta*

Basic run, output in the screen:

```
edu@somewhere:>./siesta < Fe.fdf
```

Output redirected to a file:

```
edu@somewhere:>./siesta < Fe.fdf > Fe.out
```

Screen and file output:

```
edu@somewhere: ./siesta < Fe.fdf |tee Fe.out
```

Output: the header

```
SIESTA 1.2.3 -- [iorho parallel fix/O(N)] (Nov 20, 2001)
Architecture   : lahey
Compiler flags: lf95 -O --warn --quiet --tpp --ntrace
SERIAL version

* Running in serial mode
>> Start of run:  3-JUL-2002  17:06:18
```

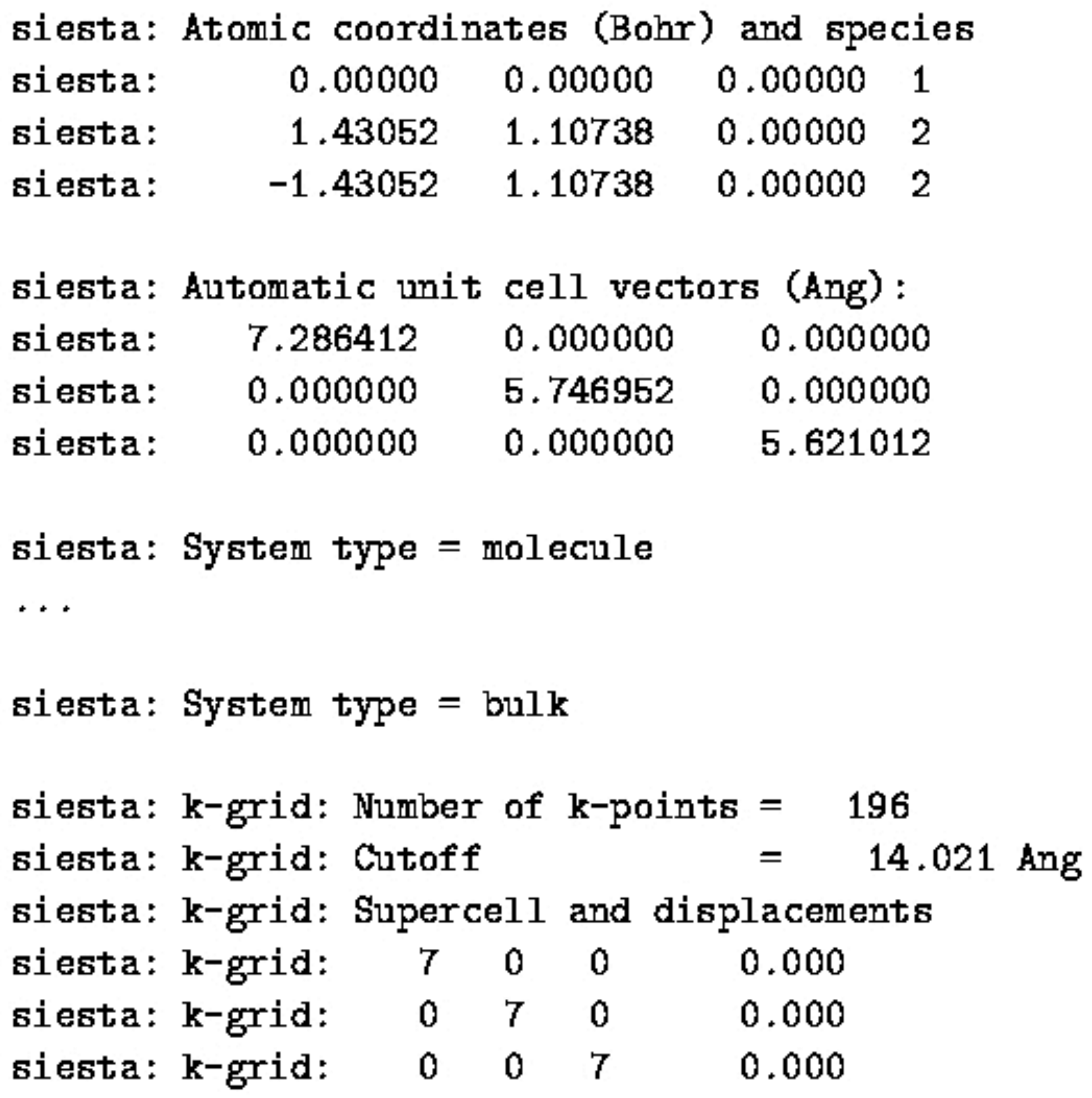
Output: dumping the input file

```
*: ****************** Dump of input data file ***********************
SystemName          Water molecule
SystemLabel         h2o
NumberOfAtoms       3
NumberOfSpecies     2
%block ChemicalSpeciesLabel
 1  8  O      # Species index, atomic number, species label
 2  1  H
%endblock ChemicalSpeciesLabel
AtomicCoordinatesFormat  Ang
%block AtomicCoordinatesAndAtomicSpecies
 0.000  0.000  0.000  1
 0.757  0.586  0.000  2
-0.757  0.586  0.000  2
%endblock AtomicCoordinatesAndAtomicSpecies
*: ****************** End of input data file ************************
```

Output: processing the input

```
prinput: *****
coor: Atomic-coordinates input format  =     Cartesian coordinates
coor:                                        (in Angstroms)
redata: Number of spin components        =     1
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: Mesh Cutoff                      =    50.0000  Ry
redata: Net charge of the system         =     0.0000 |e|
redata: Max. number of SCF Iter          =    50
redata: Mixing is linear
redata: Mix DM in first SCF step ?       =     F
redata: Write Pulay info on disk?        =     F
redata: New DM Mixing Weight             =     0.2500
redata: No kicks to SCF
redata: DM Mixing Weight for Kicks       =     0.5000
redata: DM Tolerance for SCF             =     0.000100
redata: Use continuation files for DM    =     F
redata: Neglect nonoverlap interactions  =     F
redata: Method of Calculation            =     Diagonalization
redata: Electronic Temperature           =     0.0019  Ry
redata: Fix the spin of the system       =     F
redata: Dynamics option                  =     Verlet MD run
redata: Initial MD time step             =     1
redata:   Final MD time step             =     1
redata: Length of MD time step           =     1.0000  fs
redata: Length of MD time step           =     1.0000  fs
redata: Initial Temperature of MD run    =     0.0000  K
redata: Perform a MD quench              =     F
redata: ***********************************************************
```

Output: coordinates and k-sampling



```
siesta: Atomic coordinates (Bohr) and species
siesta:       0.00000   0.00000   0.00000  1        1
siesta:       1.43052   1.10738   0.00000  2        2
siesta:      -1.43052   1.10738   0.00000  2        3

siesta: Automatic unit cell vectors (Ang):
siesta:     7.286412     0.000000     0.000000
siesta:     0.000000     5.746952     0.000000
siesta:     0.000000     0.000000     5.621012

siesta: System type = molecule
...

siesta: System type = bulk

siesta: k-grid: Number of k-points =    196
siesta: k-grid: Cutoff             =     14.021 Ang
siesta: k-grid: Supercell and displacements
siesta: k-grid:     7    0    0      0.000
siesta: k-grid:     0    7    0      0.000
siesta: k-grid:     0    0    7      0.000
```

Output: First MD step

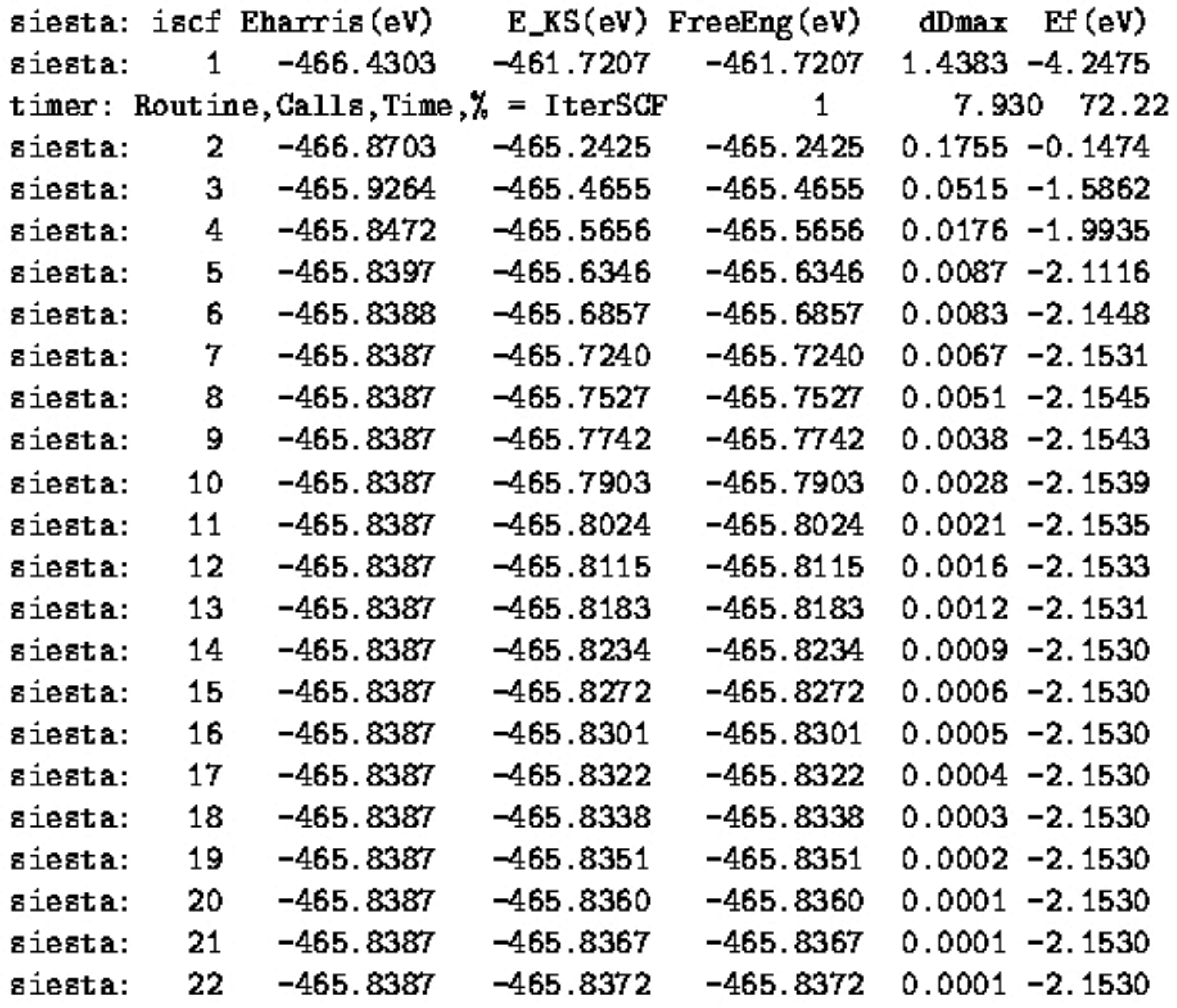
```
siesta:     ==============================
siesta:         Begin MD step =       1
siesta:     ==============================

InitMesh: MESH =    32 x    30 x    24 =       23040
InitMesh: Mesh cutoff (required, used) =    50.000    50.384 Ry

* Maximum dynamic memory allocated =     3 MB

siesta: Program's energy decomposition (eV):
siesta: Eions   =       815.854478
siesta: Ena     =       175.154399
siesta: Ekin    =       341.667405
siesta: Enl     =       -52.736793
siesta: DEna    =        -0.000001
siesta: DUscf   =         0.000000
siesta: DUext   =         0.000000
siesta: Exc     =      -109.951257
siesta: eta*DQ  =         0.000000
siesta: Emadel  =         0.000000
siesta: Eharris =      -466.430254
siesta: Etot    =      -461.720725
siesta: FreeEng =      -461.720725
```

Output: Self-consistency



```
siesta: iscf Eharris(eV)    E_KS(eV) FreeEng(eV)   dDmax  Ef(eV)
siesta:    1  -466.4303  -461.7207   -461.7207  1.4383 -4.2475
timer: Routine,Calls,Time,% = IterSCF        1       7.930  72.22
siesta:    2  -466.8703  -465.2425   -465.2425  0.1755 -0.1474
siesta:    3  -465.9264  -465.4655   -465.4655  0.0515 -1.5862
siesta:    4  -465.8472  -465.5656   -465.5656  0.0176 -1.9935
siesta:    5  -465.8397  -465.6346   -465.6346  0.0087 -2.1116
siesta:    6  -465.8388  -465.6857   -465.6857  0.0083 -2.1448
siesta:    7  -465.8387  -465.7240   -465.7240  0.0067 -2.1531
siesta:    8  -465.8387  -465.7527   -465.7527  0.0051 -2.1545
siesta:    9  -465.8387  -465.7742   -465.7742  0.0038 -2.1543
siesta:   10  -465.8387  -465.7903   -465.7903  0.0028 -2.1539
siesta:   11  -465.8387  -465.8024   -465.8024  0.0021 -2.1535
siesta:   12  -465.8387  -465.8115   -465.8115  0.0016 -2.1533
siesta:   13  -465.8387  -465.8183   -465.8183  0.0012 -2.1531
siesta:   14  -465.8387  -465.8234   -465.8234  0.0009 -2.1530
siesta:   15  -465.8387  -465.8272   -465.8272  0.0006 -2.1530
siesta:   16  -465.8387  -465.8301   -465.8301  0.0005 -2.1530
siesta:   17  -465.8387  -465.8322   -465.8322  0.0004 -2.1530
siesta:   18  -465.8387  -465.8338   -465.8338  0.0003 -2.1530
siesta:   19  -465.8387  -465.8351   -465.8351  0.0002 -2.1530
siesta:   20  -465.8387  -465.8360   -465.8360  0.0001 -2.1530
siesta:   21  -465.8387  -465.8367   -465.8367  0.0001 -2.1530
siesta:   22  -465.8387  -465.8372   -465.8372  0.0001 -2.1530
```

Output: Eigenvalues, forces, stress

```
siesta: Eigenvalues (eV):
  ik is     eps
   1  1 -24.74 -12.70  -8.71  -6.23   1.68   4.09
         14.68  21.97  24.22  27.21  28.65  32.19
         49.89  70.65  96.18

siesta: Atomic forces (eV/Ang):
siesta:     1     0.000001   -0.504870    0.000000
siesta:     2     0.719664    0.279830    0.000000
siesta:     3    -0.719663    0.279829    0.000000
siesta: ----------------------------------------
siesta:   Tot     0.000002    0.054788    0.000000

siesta: Stress tensor (eV/Ang**3):
siesta:     -0.012622    0.000000    0.000000
siesta:      0.000000   -0.002309    0.000000
siesta:      0.000000    0.000000    0.014000
```

Output: Total energy

```
siesta: Fermi energy =      -2.152975 eV

siesta: Program's energy decomposition (eV):
siesta:-Eions   =     -815.854478
siesta: Ena     =      175.154399
siesta: Ekin    =      350.784945
siesta: Enl     =      -61.958840
siesta: DEna    =       -1.777979
siesta: DUscf   =        0.727284
siesta: DUext   =        0.000000
siesta: Exc     =     -112.912881
siesta: eta*DQ  =        0.000000
siesta: Emadel  =        0.000000
siesta: Ekinion =        0.000000
siesta: Eharris =     -465.839084
siesta: Etot    =     -465.837551
siesta: FreeEng =     -465.837551

siesta: Final energy (eV):
siesta:       Kinetic =     350.784945
siesta:       Hartree =     382.616610
siesta:    Ext. field =       0.000000
siesta:   Exch.-corr. =    -112.912881
siesta:  Ion-electron =   -1072.820417
siesta:       Ion-ion =     -13.505807
siesta:       Ekinion =       0.000000
siesta:         Total =    -465.837551
```

Output: timer (real and cpu times)

```
timer: CPU execution times:
timer:  Routine    Calls Time/call  Tot.time       %
timer:  siesta         1    13.660    13.660  100.00
timer:  Setup          1     0.850     0.850    6.22
timer:  bands          1     0.000     0.000    0.00
timer:  KSV_init       1     0.000     0.000    0.00
timer:  IterMD         1    12.800    12.800   93.70
timer:  hsparse        2     0.005     0.010    0.07
timer:  overfsm        2     1.095     2.190   16.03
timer:  IterSCF       23     0.461    10.600   77.60
timer:  kinefsm        2     1.010     2.020   14.79
timer:  nlefsm         2     2.780     5.560   40.70
timer:  DHSCF         23     0.128     2.950   21.60
timer:  DHSCF1         1     0.060     0.060    0.44
timer:  DHSCF2         1     0.190     0.190    1.39
timer:  REORD        186     0.001     0.130    0.95
timer:  POISON        24     0.020     0.480    3.51
timer:  DHSCF3        23     0.110     2.520   18.45
timer:  rhoofd        23     0.030     0.690    5.05
timer:  CELLXC        23     0.027     0.610    4.47
timer:  vmat          23     0.018     0.410    3.00
timer:  diagon        22     0.002     0.050    0.37
timer:  rdiag         22     0.002     0.040    0.29
timer:  DHSCF4         1     0.180     0.180    1.32
timer:  dfscf          1     0.150     0.150    1.10

>> End of run:   3-JUL-2002   17:06:32
```

Saving and reading information (I)

Some information is stored by Siesta to restart simulations from:

- •Density matrix: DM.UseSaveDM
- •Localized wave functions (Order-N): ON.UseSaveLWF
- •Atomic positions and velocities: MD.UseSaveXV
- •Conjugent gradient history (minimizations): MD.UseSaveCG

All of them are logical variables

EXTREMLY USEFUL TO SAVE LOT OF TIME!

Saving and reading information (II)

Information needed as input for various post-processing programs, for example, to visualize:

- Total charge density: SaveRho
- Deformation charge density: SaveDeltaRho
- Electrostatic potential: SaveElectrostaticPotential
- Total potential: SaveTotalPotential
- Local density of states: LocalDensityOfStates
- Charge density contours: WriteDenchar
- Atomic coordinates: WriteCoorXmol and WriteCoorCerius

All of them are logical variables

Analyzing the electronic structure (I)

•**Band structure** along the high symetry lines of the BZ

BandLineScale: scale of the k vectors in BandLines

```
BandLineScale      pi/a
```

BandLines: lines were band energies are calculated.

```
%block BandLines
1     1.000    1.000   1.000    L
20   0.000    0.000   0.000    \Gamma
25   2.000    0.000   0.000   X
30   2.000    2.000   2.000 \Gamma
%endblock BandLines
```

Analyzing the electronic structure (II)

•**Density of states**: total and projected on the atomic orbitals

- Compare with experimental spectroscopy

- Bond formation

- Defined as:

$$g\left(\epsilon\right) = \sum_{i}\sum_{\mathbf{k}} \delta\left(\epsilon - \epsilon_i\left(\mathbf{k}\right)\right)$$
$$\simeq \sum_{i}\sum_{\mathbf{k}} \frac{1}{\sigma\sqrt{\pi}} exp\left(-\frac{\left(\epsilon - \epsilon_i\left(\mathbf{k}\right)\right)^2}{\sigma^2}\right)$$

ProjectedDensityOfStates:

```
%block ProjectedDensityOfStates
-20.00   10.00   0.200  500  eV
%endblock ProjectedDensityOfStates
```

Analyzing the electronic structure (III)

•**Population analysis: Mulliken** prescription

- Amounts of charge on an atom or in an orbital inside the atom

- Bond formation

- Be careful, very dependent on the basis functions

WriteMullikenPop

```
WriteMullikenPop    0  = None
                    1  = Atomic and orbitals charges
                    2  = 1 + atomic overlap pop.
                    3  = 2 + orbital overlap pop.
```

Tools (I)

•Various **post-processing programs**:

-PHONONS:

-Finite differences: VIBRA (P. Ordejón)

-Linear response: LINRES (J. M. Alons-Pruneda et al.)

-Interphase with Phonon program (Parlinsky)

-Visualize of the CHARGE DENSITY and POTENTIALS

-3D: PLRHO (J. M. Soler)

-2D: CONTOUR (E. Artacho)

-2D: DENCHAR (J. Junquera)

-3D: sies2xsf (Xcrysden) (A. Postnikov: Friday 11:15)

-3D: grid2cube (Gaussian) (P. Ordejón)

-3D: rho2grd (Materials Studio) (O. Paz)

Tools (II)

-TRANSPORT PROPERTIES:

-TRANSIESTA (M. Brandbydge *et al*.)

-PSEUDOPOTENTIAL and BASIS information:

-PyAtom (A. García)

-ATOMIC COORDINATES:

-Sies2arc (J. Gale)

– DOS, PDOS, Bands:

-PlotUtils (O. Paz)