SUMMER SCHOOL ON COMPUTATIONAL MATERIALS SCIENCE

University of Illinois at Urbana-Champaign, June 13-23, 2005

How to run SIESTA

Introduction to input & output files

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

- Born-Oppenheimer
- DFT
- Pseudopotentials
- Numerical atomic orbitals
- Numerical evaluation of matrix elements

- *relaxations, MD, phonons.*
- *LDA, GGA*
- *norm conserving, factorised.*
- *finite range*

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)

What do we need?

- Access to the executable file: siesta
- An input file
  - Flexible Data Format (fdf) *(A. García & J.M. Soler).*
- A psedopotential file for each kind of element in the input file.
  - Unformatted binary (vps)
  - Formatted ASCII (.psf): more transportable and readable

Siesta package: (under license)

- Src: Sources of the Siesta code
- Docs: Documentation and user conditions
    - User’s Guide (siesta.tex)
- Pseudo: ATOM program to generate and test pseudopotentials
- Examples: fdf and pseudopotentials input files for simple systems
- Utils: Programs or scripts to analyze the results

The input file

- Main input file:
    - Flexible Data Format (FDF)
    - Physical data of the system
    - Variables to control the approximations

FDF characteristics (II)

- Data can be given in any order
- Data can be omitted in favour of *default* values.
- Labels are case insensitive and characters `-´ , `_´, `.´ are ignored:

  LatticeConstant is equivalent to lattice_constant

- Text following # are comments
- You may 'include' other FDF files or redirect the search to another file

FDF characteristics (II)

- 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

- Physical magnitudes: followed by their units.

Many units are valid for the same magnitude (m, cm, nm, Ang, Bohr).
There is an automatic conversion to the units required internally.

- Character strings, NOT in apostrophes

FDF characteristics (III)

- Logical values: T / .true. / true / yes

  F / .false. / false / no

- Complex data structures: *blocks*

  %block label

  …

  %endblock label

Basic input variables

a) General system descriptors

b) Structural and geometrical variables

c) Functional and solution mehod

d) Convergence of the results

e) Self-consistency

f) Basis set generation related variables.

General System description

SystemName: descriptive name of the system

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

SystemLabel: nickname to label output files

```
SystemLabel         silicon
```

After a succesful run, you should have files like

silicon.DM : *Density matrix*

silicon.XV : *Final positions and velocities*

silicon.EIG : *Eigen-energies*

…

Geometrical and structural 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

LatticeConstant: length to define the scale of the lattice vectors

```
LatticeConstant                5.43 Ang
```

LatticeParameters: Crystallograhic way

```
%block LatticeParameters
  1.0   1.0   1.0   60.0   60.0   60.0
%endblock LatticeParameters
```

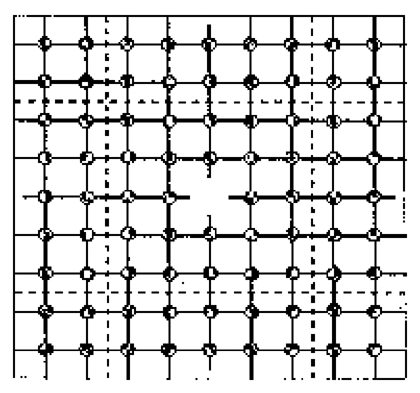
LatticeVectors: read as a matrix, each vector being a line

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

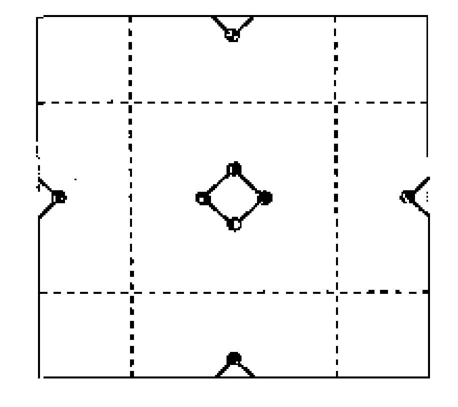
Periodic Boundary Conditions (PBC)

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

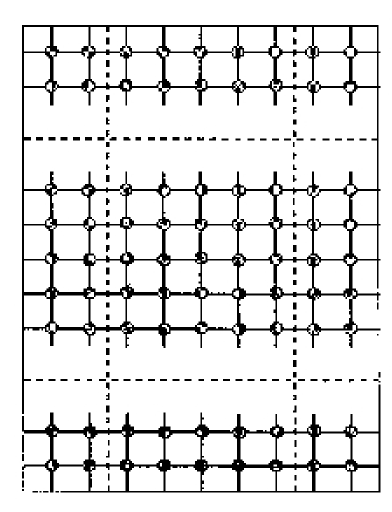
- Periodic systems and crystalline solids: √
- Aperiodic systems: *Supercell approximation*



Defects



Molecules



Surfaces

Atomic Coordinates

AtomicCoordinatesFormat: format of the atomic positions in input:

Bohr: cartesian coordinates, in bohrs

Ang: cartesian coordinates, in Angstroms

ScaledCartesian: cartesian coordinates, units of the lattice constant

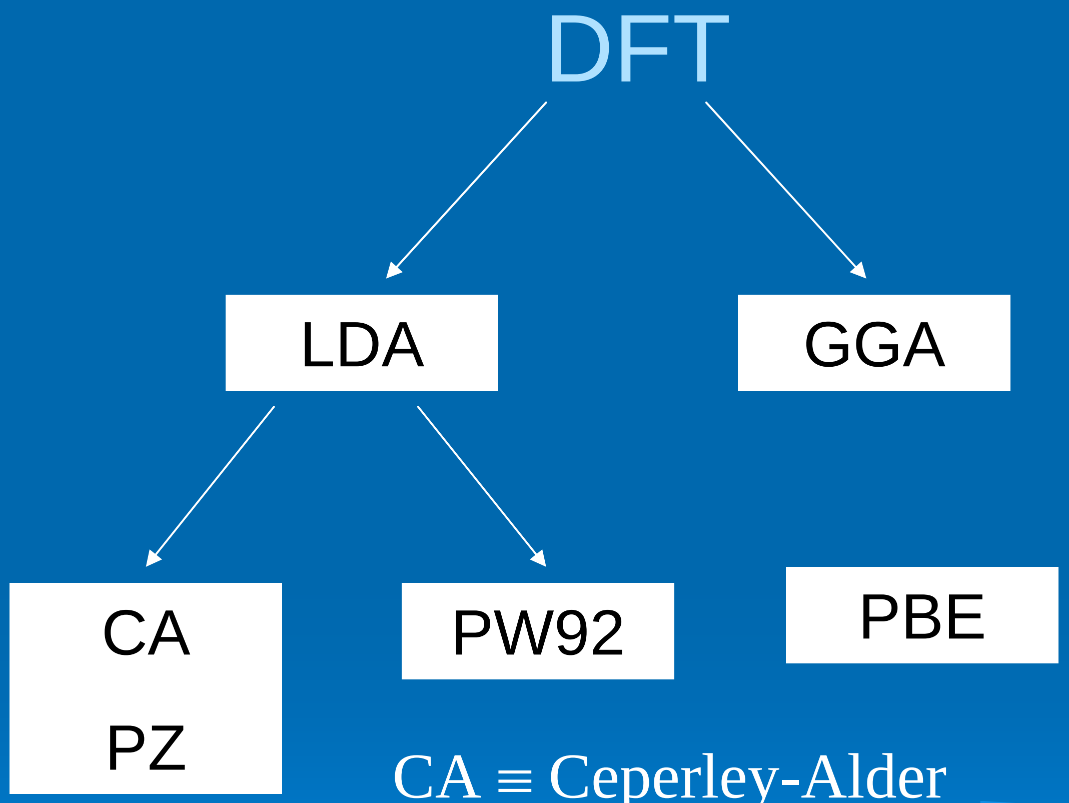
Fractional: referred to the lattice vectors

```
AtomicCoordinatesFormat         Fractional
```

AtomicCoordinatesAndAtomicSpecies:

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

XC-functional



DFT

XC.Functional

LDA

GGA

XC.authors

CA

PZ

PW92

PBE

SpinPolarized

CA ≡ Ceperley-Alder

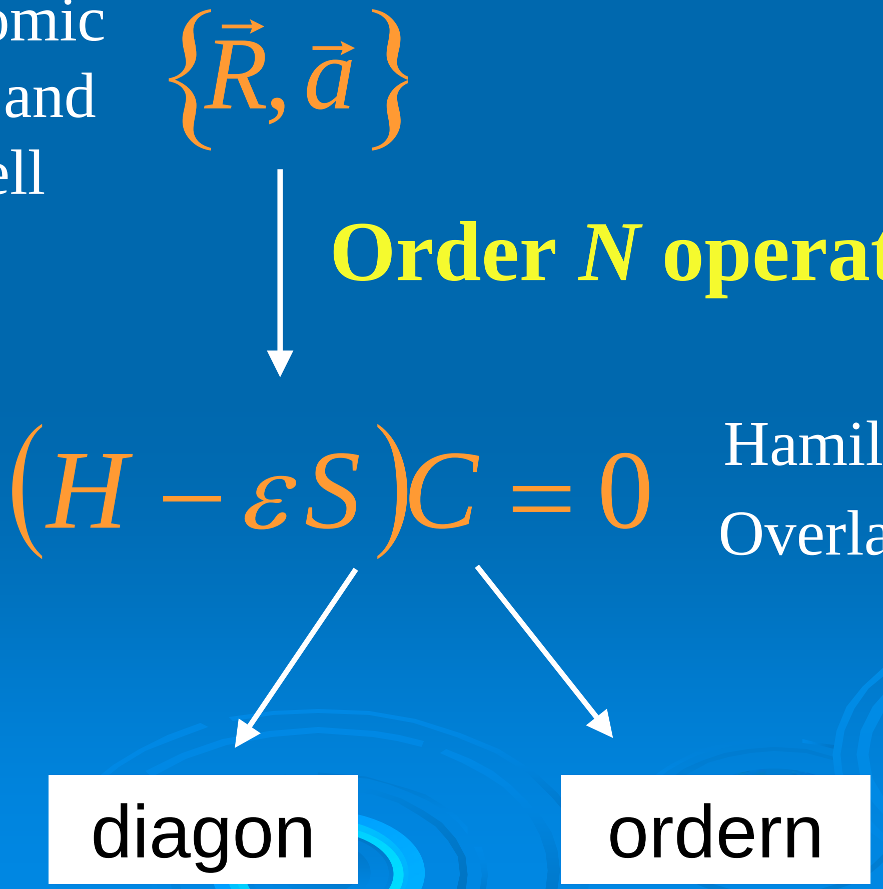
PZ ≡ Perdew-Zunger

PW92 ≡ Perdew-Wang-92

PBE ≡ Perdew-Burke-Ernzerhof

Solution method

Two options to solve the electronic problem (Kohn-Sham equations)



From the atomic coordinates and the unit cell

$$\left\{\vec{R},\vec{a}\,\right\}$$

Order *N* operations

$$\left(H-\varepsilon S\right)C=0$$

Hamiltonian, ***H***, and Overlap, ***S***, matrices

SolutionMethod

diagon

ordern

K-point sampling

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

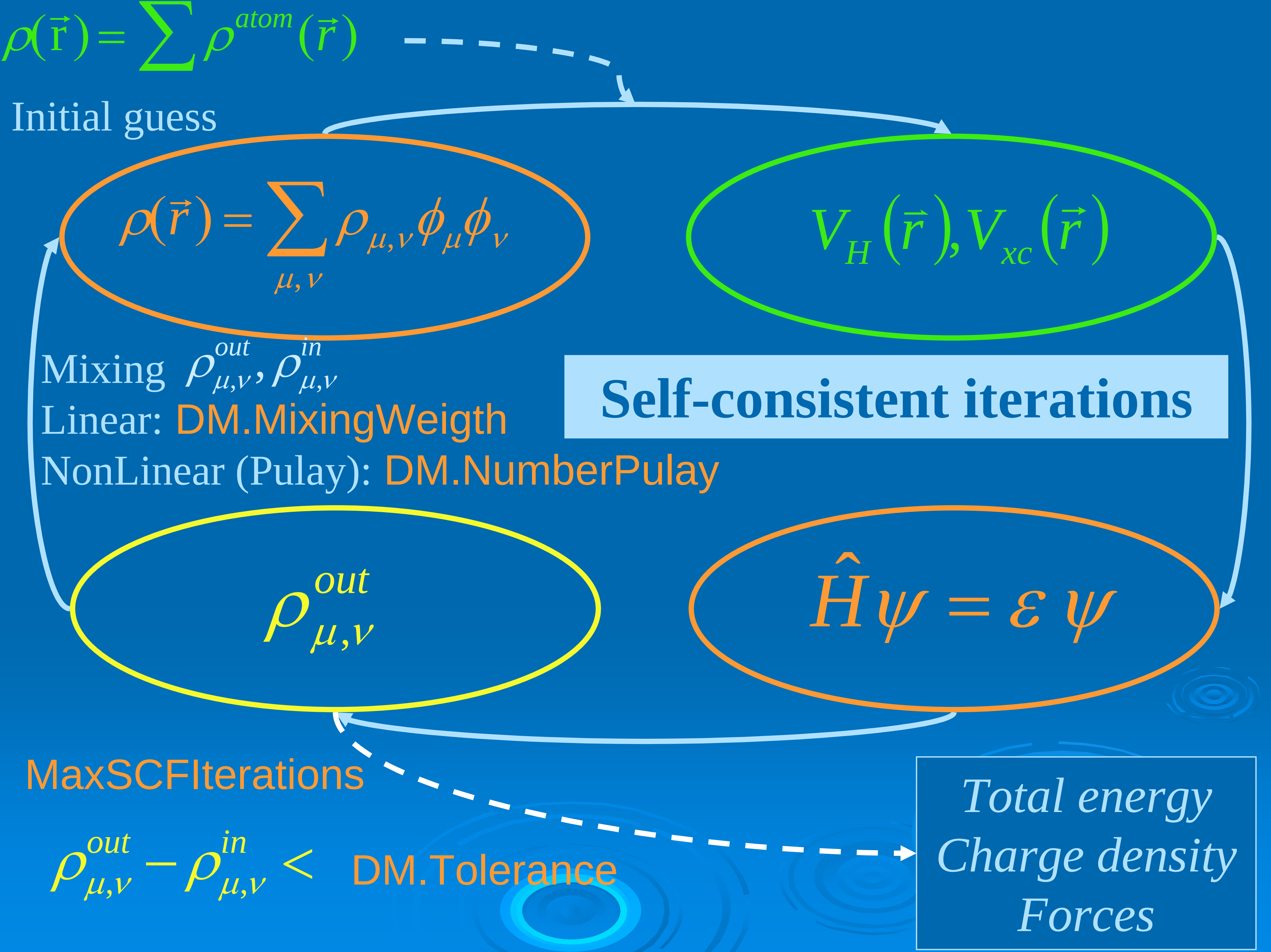
Baldereschi, Chadi-Cohen, Monkhorst-Pack

kgrid_cutoff:

```
Kgrid_cutoff            10.0 Ang
```

kgrid_Monkhorst_Pack:

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



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

Initial guess

$$\rho(\vec{r}) = \sum_{\mu,\nu} \rho_{\mu,\nu} \phi_\mu \phi_\nu$$

$$V_H(\vec{r}), V_{xc}(\vec{r})$$

Mixing $\rho^{out}_{\mu,\nu}, \rho^{in}_{\mu,\nu}$

Linear: DM.MixingWeigth

NonLinear (Pulay): DM.NumberPulay

Self-consistent iterations

$$\rho^{out}_{\mu,\nu}$$

$$\hat{H}\psi = \varepsilon\,\psi$$

MaxSCFIterations

$\rho^{out}_{\mu,\nu} - \rho^{in}_{\mu,\nu} <$ DM.Tolerance

Total energy

Charge density

Forces

How to run siesta

- To run the serial version:

```
[path]/siesta < input.fdf > output &
```

- To see the information dumbed in the output file while it runs

```
tail –f output
```

- Alternatively:

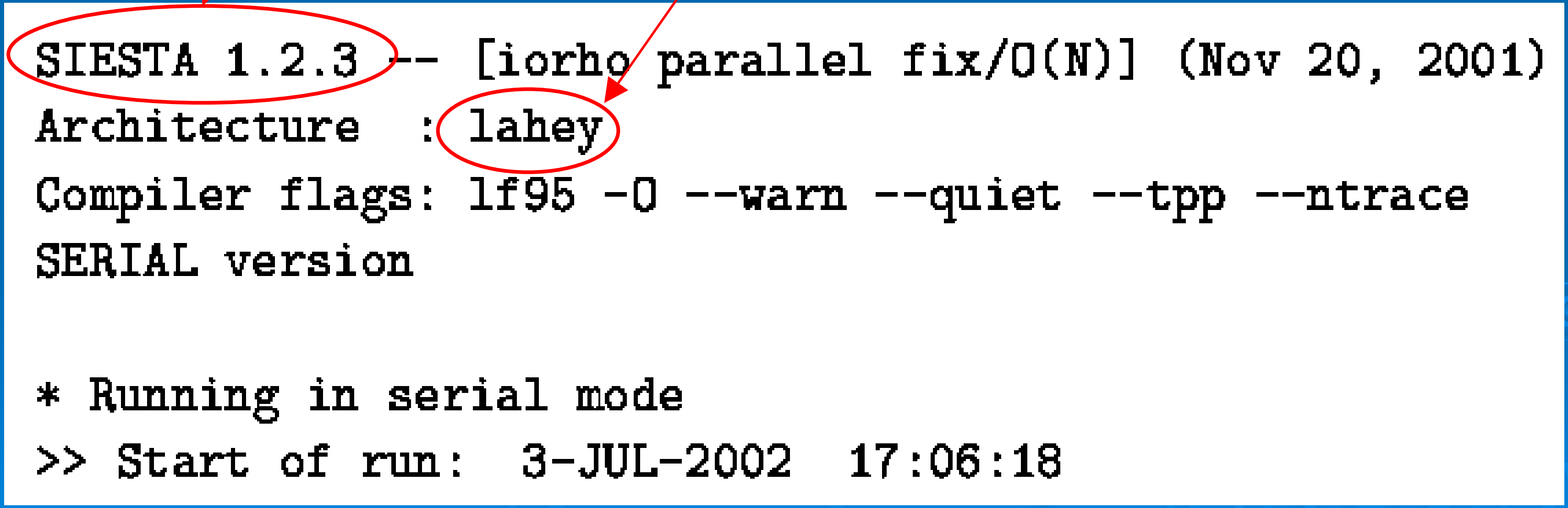
```
[path]/siesta < input.fdf | tee ouput
```

Analysing the output (I)

The output header

Siesta version

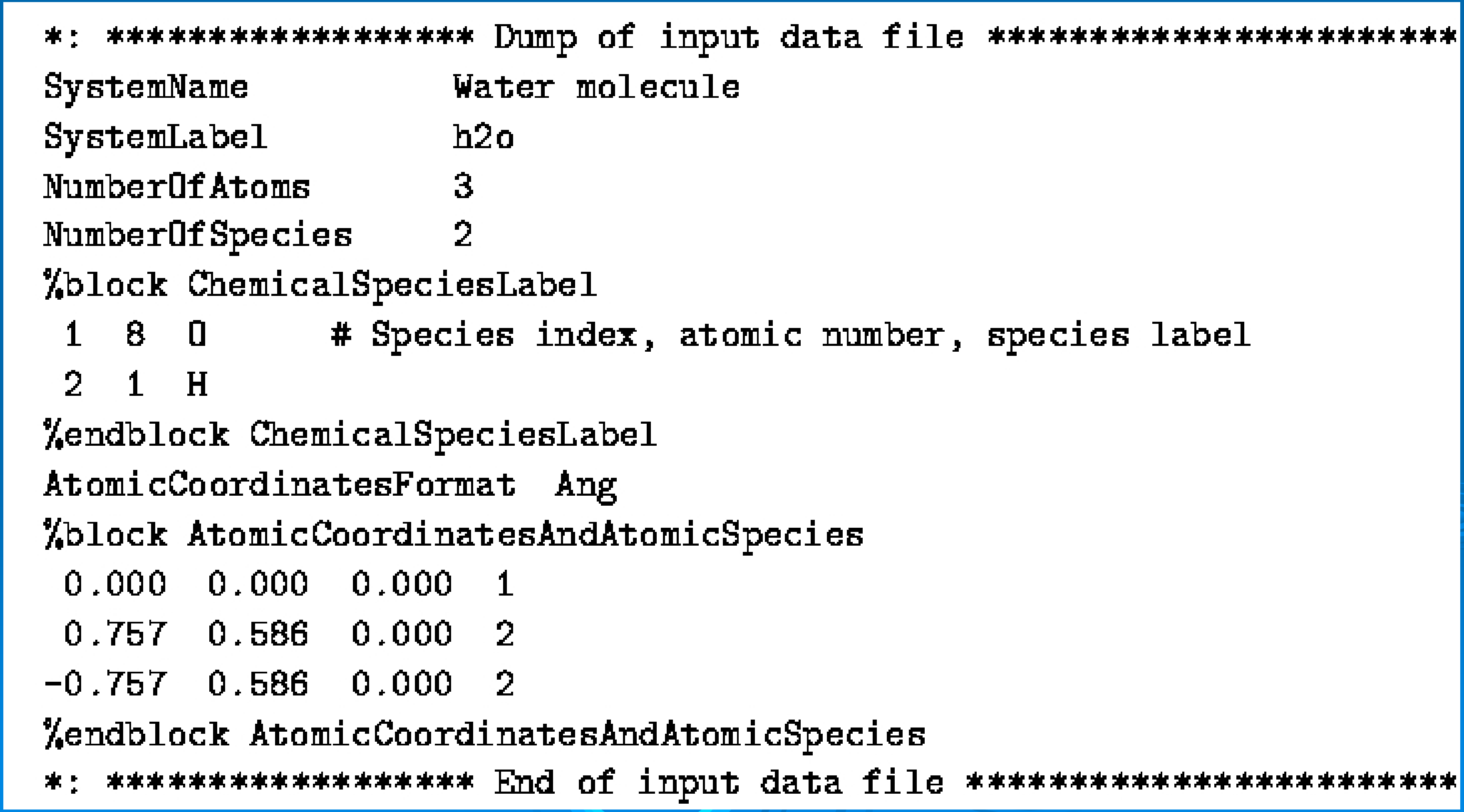
Fortran compiler



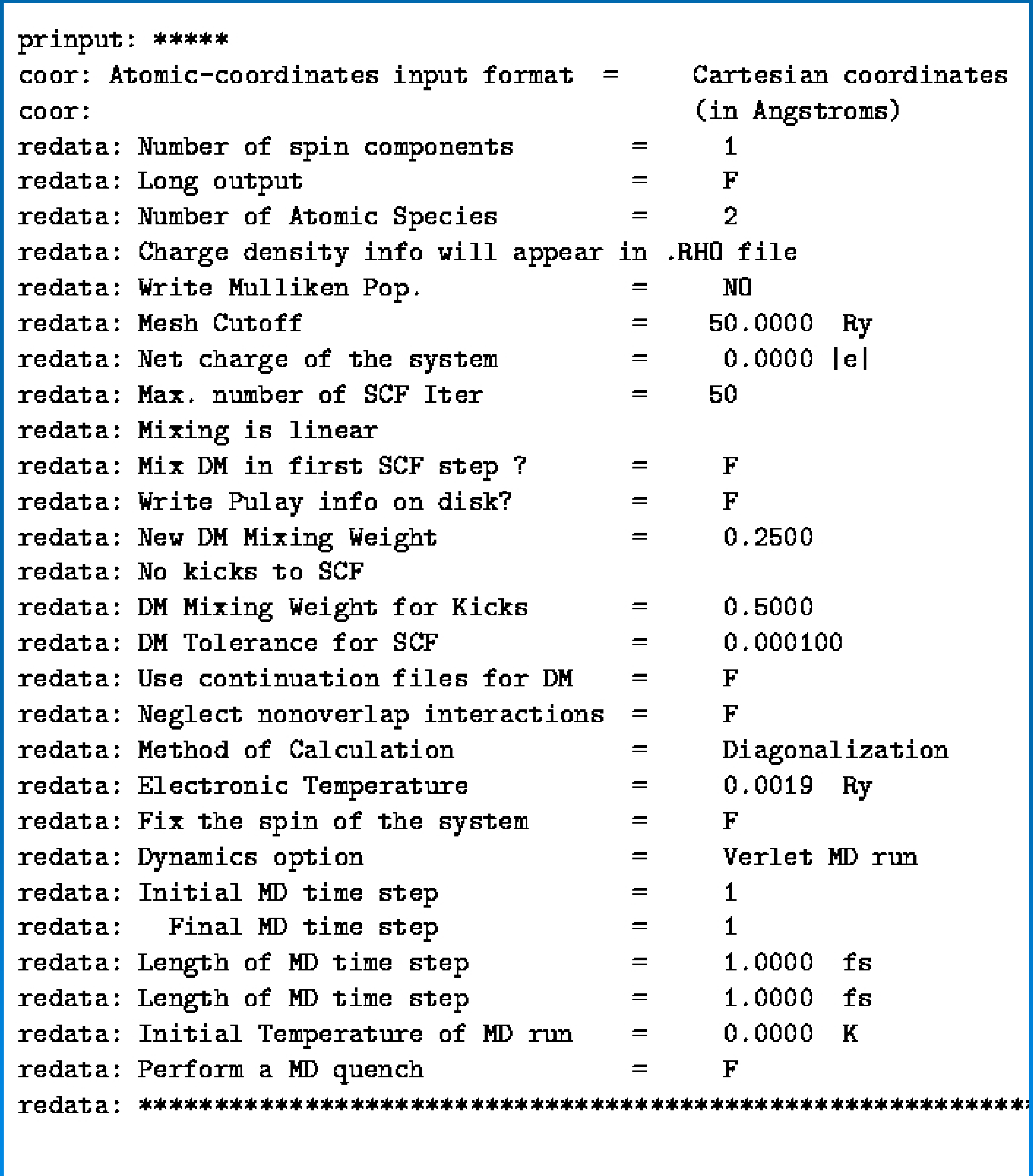
```
SIESTA 1.2.3 -- [iorho parallel fix/O(N)] (Nov 20, 2001)
Architecture  : lahey
Compiler flags: lf95 -O --warn --quiet --tpp --ntrace
SERIAL version


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

Analysing the output (II)

dumping the input file



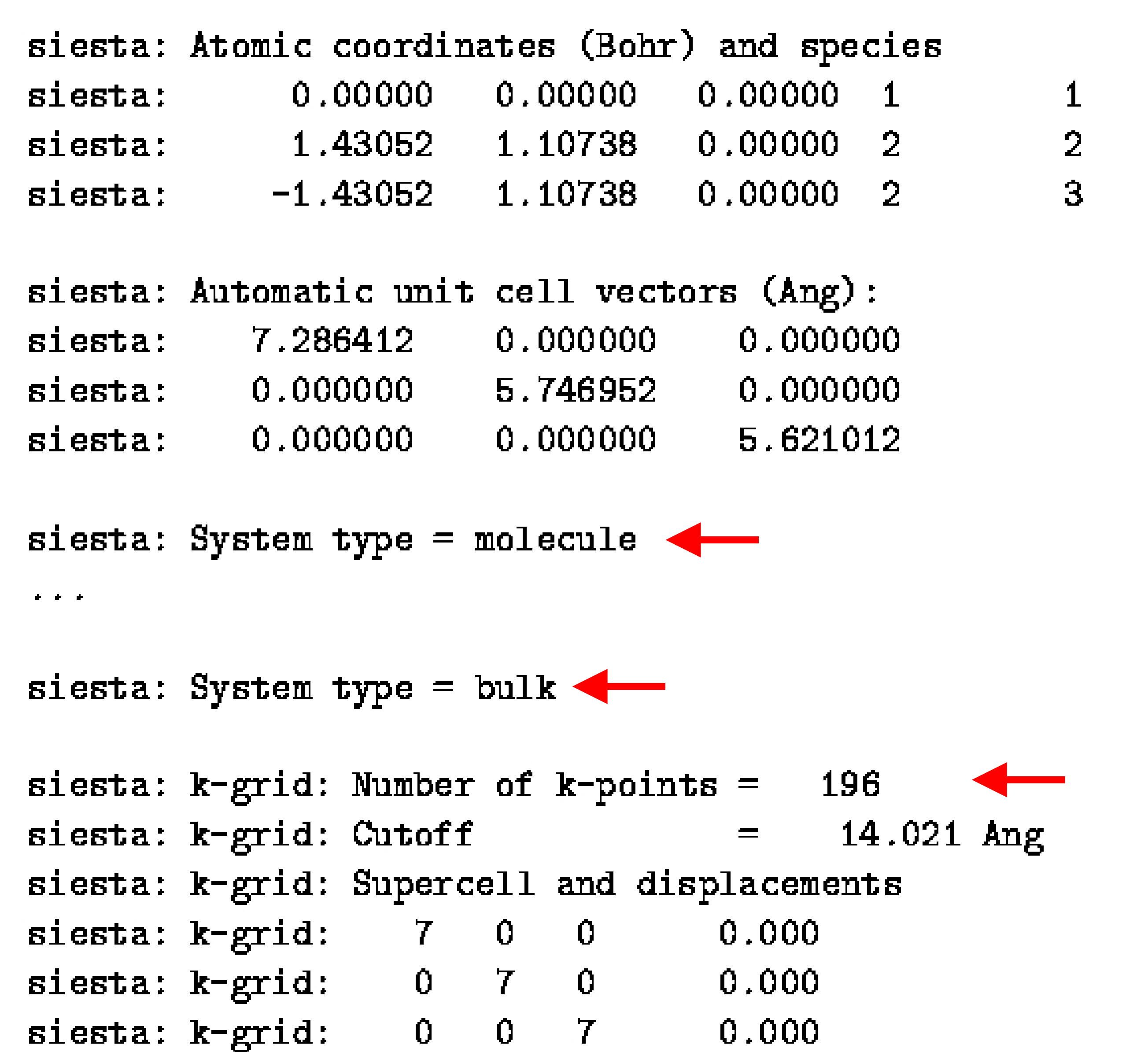
```
*: ****************** Dump of input data file ***********************
SystemName              Water molecule
SystemLabel             h2o
NumberOfAtoms           3
NumberOfSpecies         2
%block ChemicalSpeciesLabel
 1  8  O      # Species index, atomic number, species label
 2  1  H
%endblock ChemicalSpeciesLabel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



```
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: ******************************************************************
```

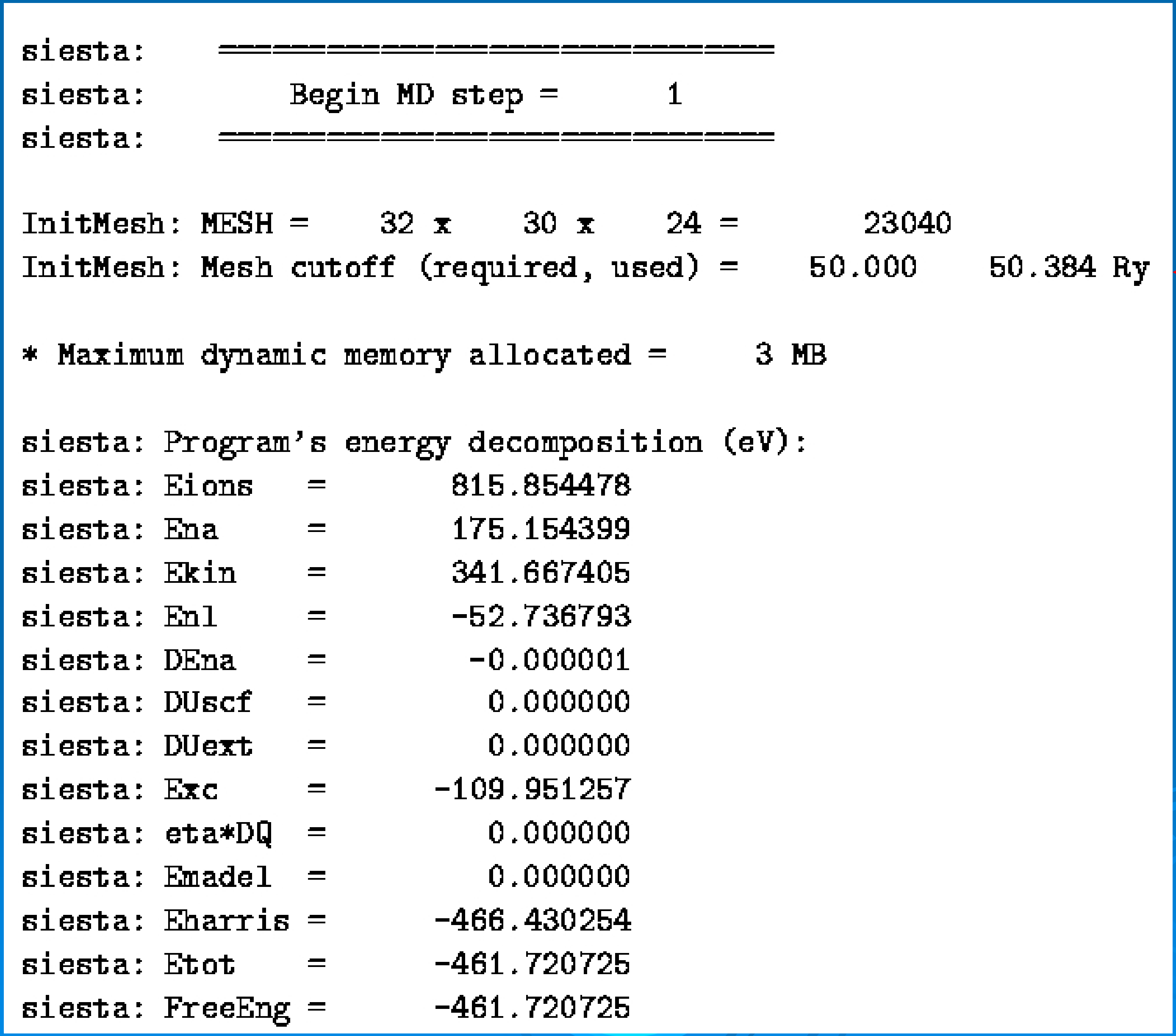
processing the input

coordinates and k-sampling



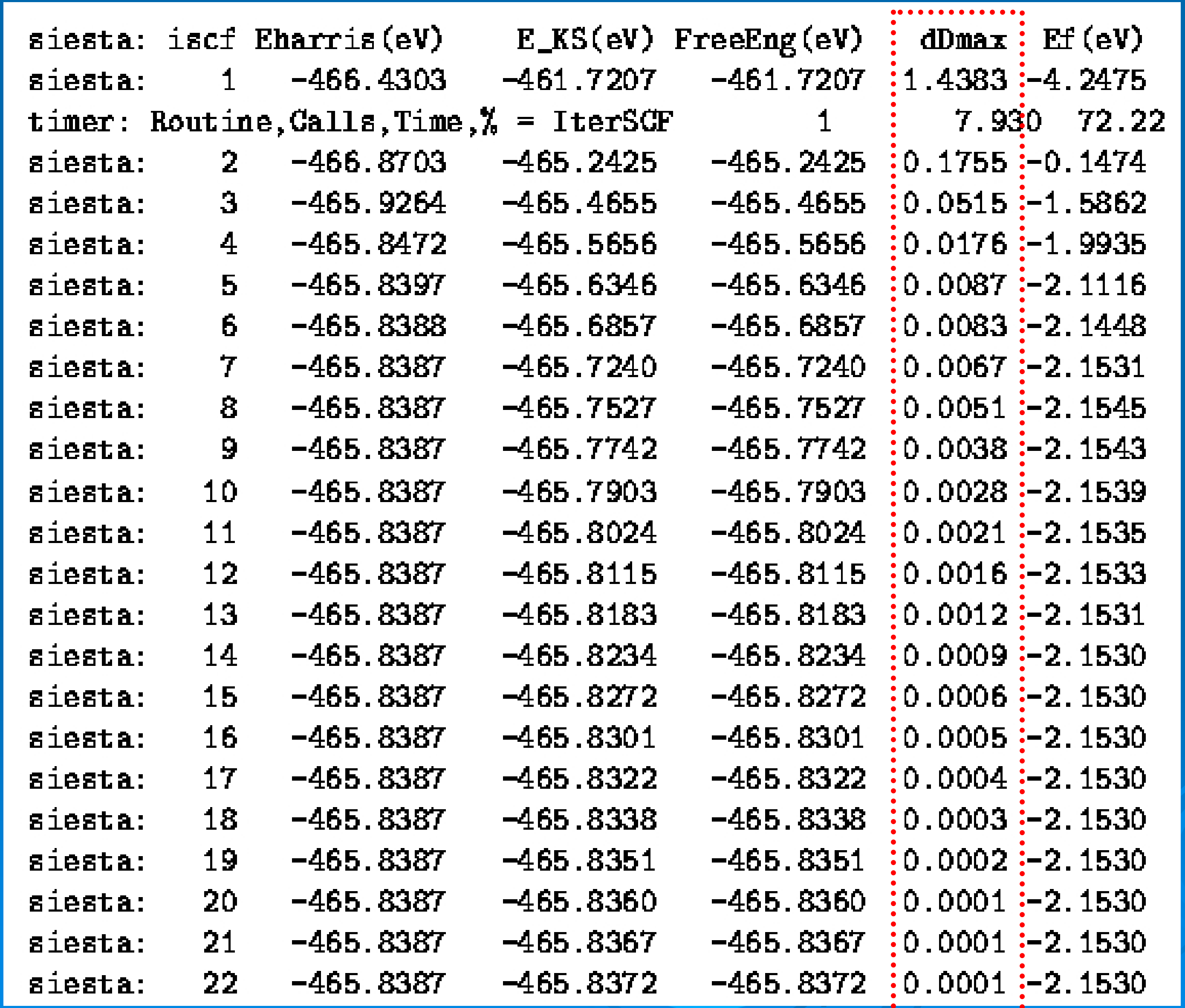
```
siesta: Atomic coordinates (Bohr) and species
siesta:       0.00000   0.00000   0.00000  1        1
siesta:       1.43052   1.10738   0.00000  2        2
siesta:      -1.43052   1.10738   0.00000  2        3

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



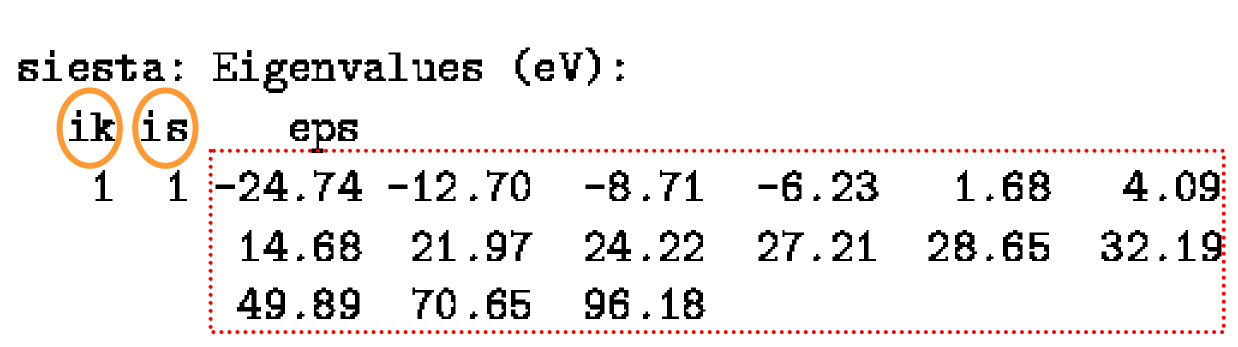
```
siesta:    ===============================
siesta:        Begin MD step =      1
siesta:    ===============================

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

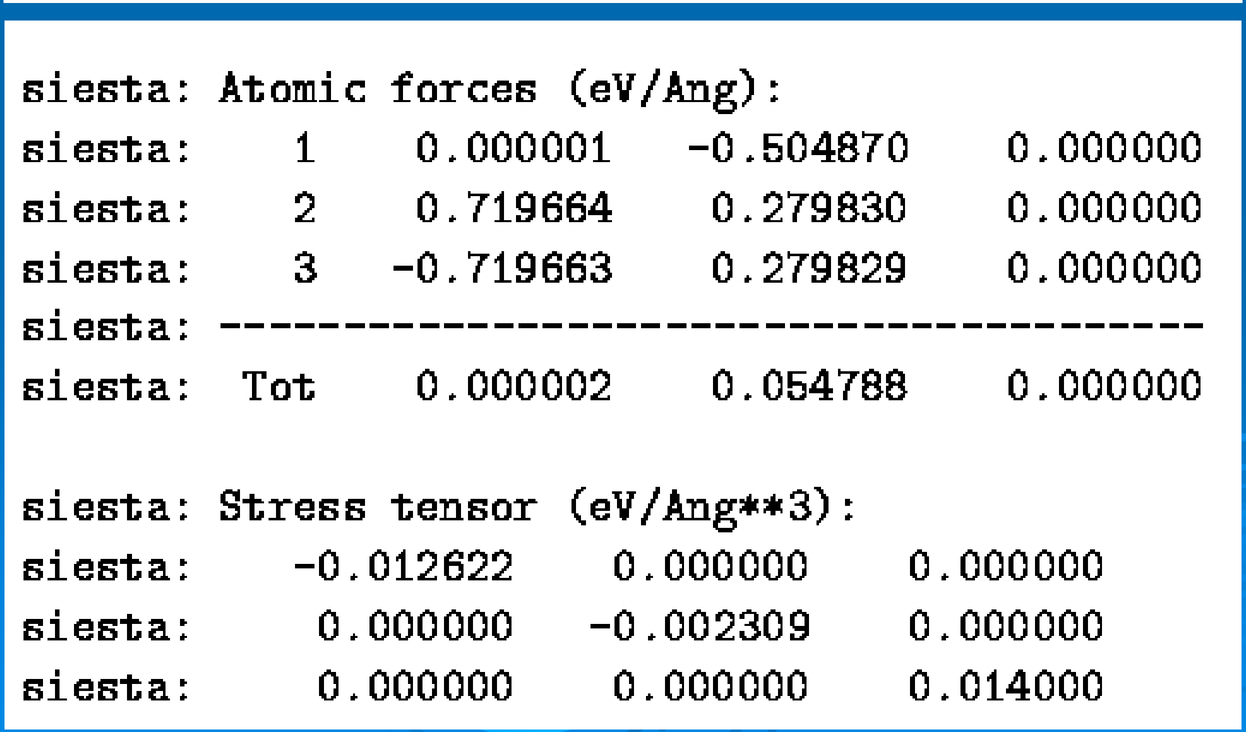


```
siesta: iscf Eharris(eV)     E_KS(eV)  FreeEng(eV)   dDmax   Ef(eV)
siesta:    1   -466.4303   -461.7207   -461.7207  1.4383 -4.2475
timer: Routine,Calls,Time,% = IterSCF        1       7.930   72.22
siesta:    2   -466.8703   -465.2425   -465.2425  0.1755 -0.1474
siesta:    3   -465.9264   -465.4655   -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

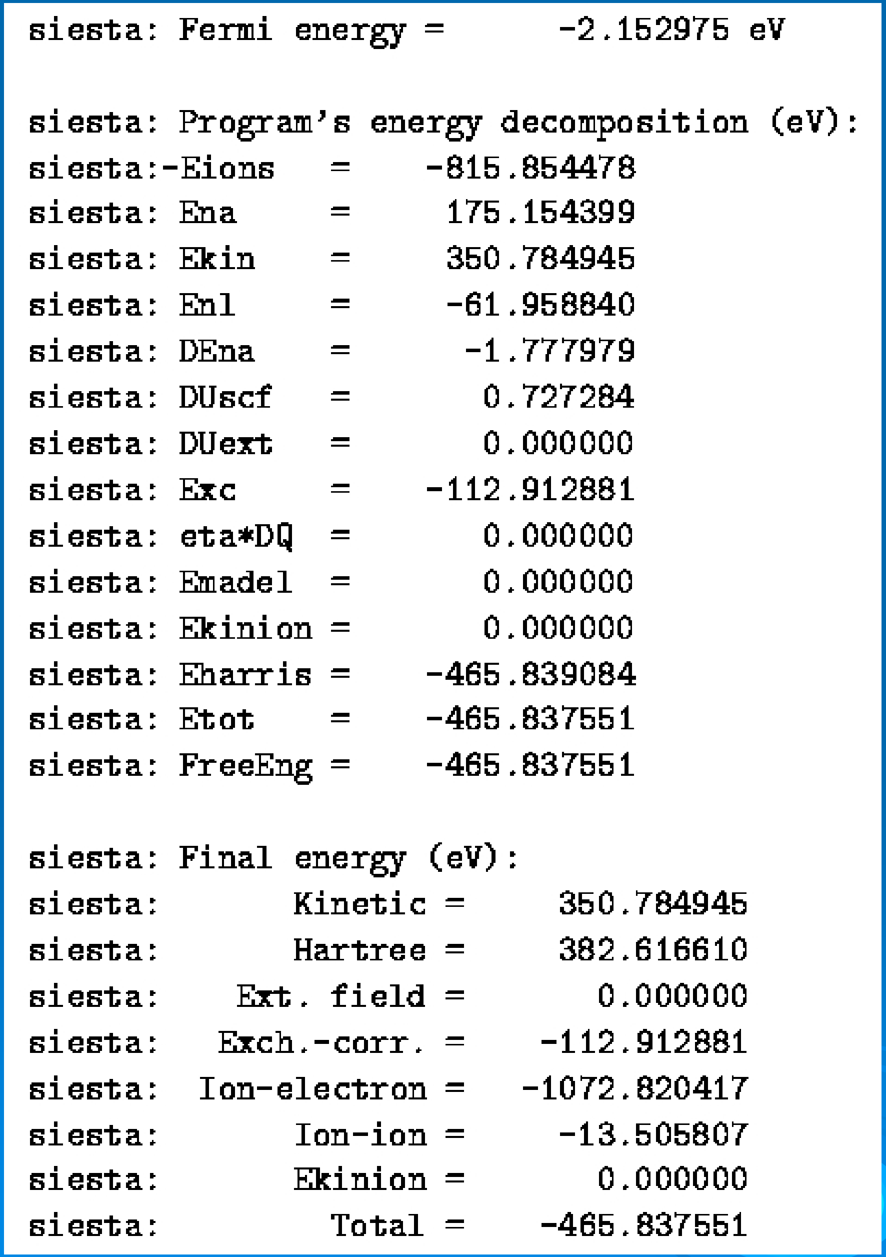


```
siesta: Eigenvalues (eV):
  ik is     eps
   1  1 -24.74 -12.70  -8.71  -6.23   1.68   4.09
         14.68  21.97  24.22  27.21  28.65  32.19
         49.89  70.65  96.18
```



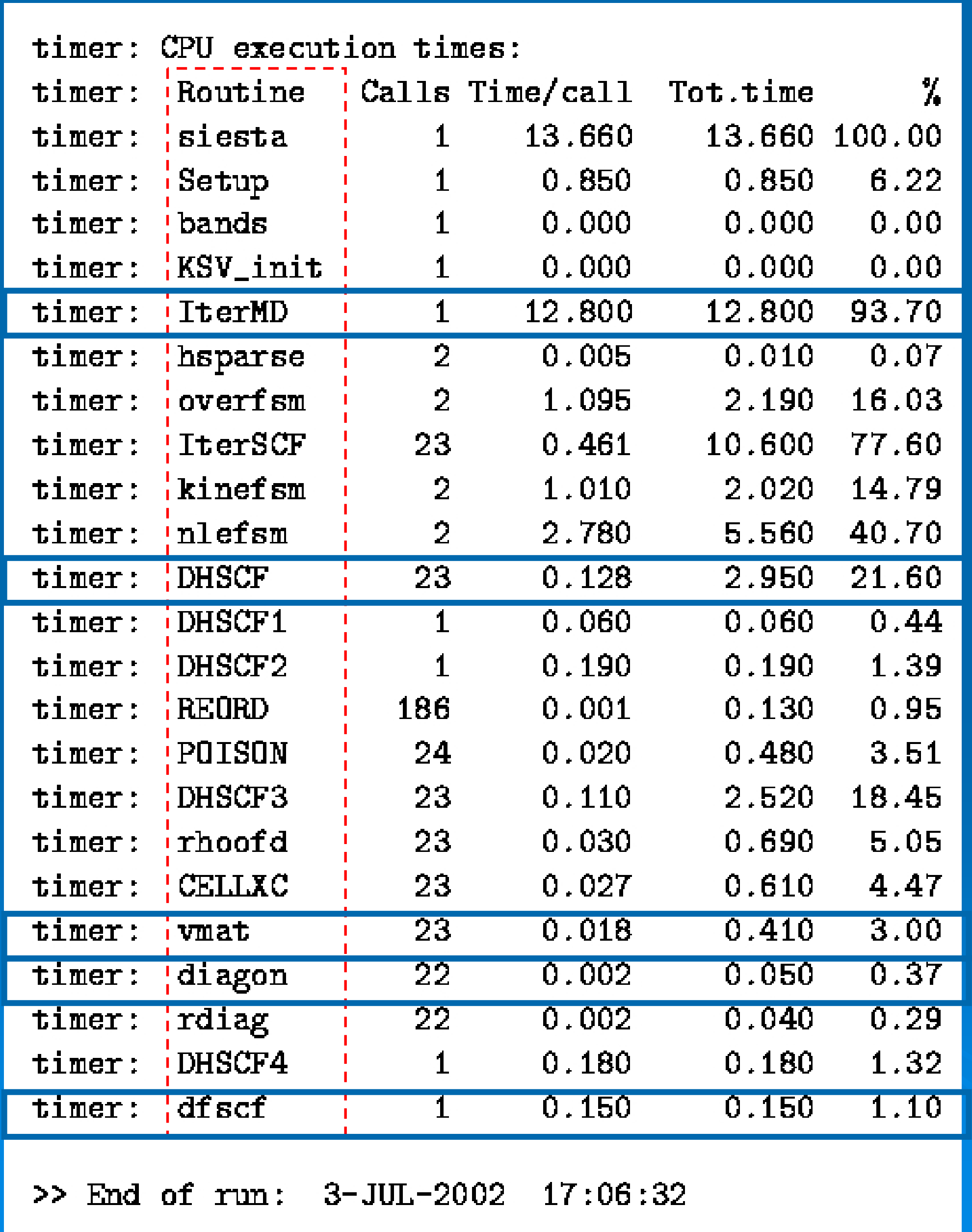
```
siesta: Atomic forces (eV/Ang):
siesta:     1    0.000001   -0.504870    0.000000
siesta:     2    0.719664    0.279830    0.000000
siesta:     3   -0.719663    0.279829    0.000000
siesta: ----------------------------------------
siesta:   Tot    0.000002    0.054788    0.000000

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



```
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 & reading information (I)

Some information is stored by Siesta and can be used to restart the simulations from previous a run:

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

All of them are logical variables *(and save lots of time!!)*

Saving & 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

```
BandLinesScale      pi/a
```

  - BandLines: lines along with 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

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

- ProjectedDensityOfStates:

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

Lower energy   Higher energy   width   # points

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

Utilities (I)

Various post-processing tools:

- PHONONS:
  - Finite differences: VIBRA (P. Ordejón)
  - Linear response: LINRES (M. Pruneda et al.)
  - Interphase with Phonon program (Parlinsky)

- Visualization of the CHARGE DENSITY and POTENTIALS
  - -3D: PLRHO (J. M. Soler), grid2cube, grid2xfs, …
  - -2D: CONTOUR (E. Artacho)
  - -2D: DENCHAR (J. Junquera)

Utilities (II)

- TRANSPORT PROPERTIES:
  - TRANSIESTA (M. Brandbydge *et al*.),
  - SMEAGOL (S. Sanvito *et. al.*)
- PSEUDOPOTENTIAL and BASIS information:
  - PyAtom (A. García).
- XML output:
  - Visualization of the ouput (J. Wakelin & A. García).
  - PDOS-xml tool (A. García)
- ATOMIC COORDINATES:
  - Sies2arc (J. Gale)