Example I: Total energy of S_2 dimer within LDA approximation

In this example we will calculate the total energy of the S_2 dimer using LDA approximation for the exchange-correlation functional.
Let us look at the input file

The first directive "echo" is optional but highly recommended. Its purpose is to write out the contents of your input file into the output file.

echo

The "title" is also optional. You might want to put a short sentence identifying the nature of your calculation .

title "total energy of s2-dimer LDA/30Ry with PSPW method"

The "start" directive is required. It indicates that this is a new calculation and sets up the name of the database to store your results.

start s2-pspw-energy

The name of the database file that you would like to associate with this calculation

scratch_dir ./scratch
permanent_dir ./perm

The location of permanent and scratch directories. The scratch directory contains temporary files. The permanent directory contains essential files which will be required should you wish to restart your calculation
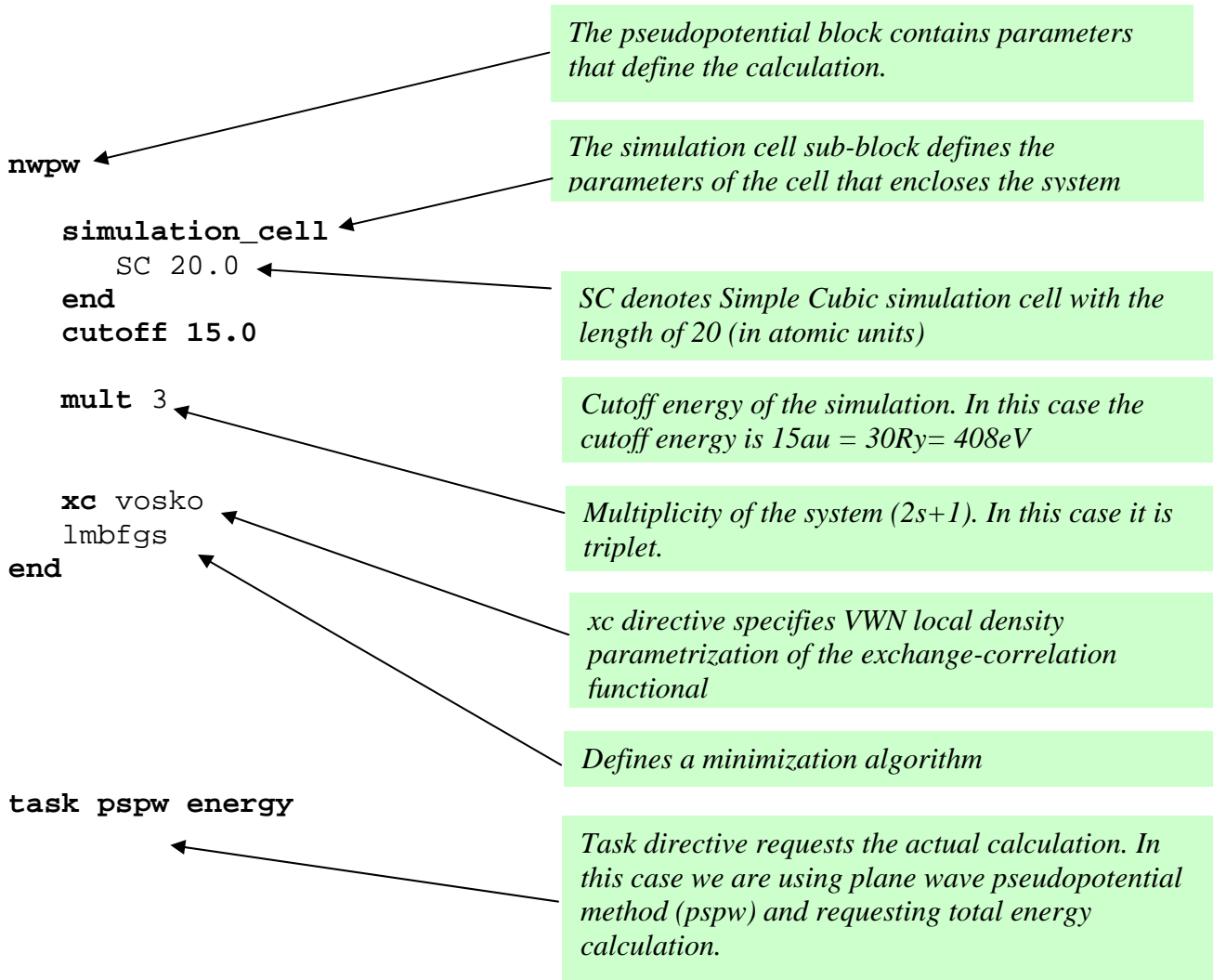
geometry
S 0.0 0.0 0.0
S 0.0 0.0 1.88
end

The geometry block specifies the name of the elements that comprise your system as well as their coordinates in the following format:
Name1 x1 y1 z1
Name2 x2 y2 z2
……
Unless indicated otherwise the default units are angstroms, and the system will be centered around the origin.

```
                nwpw

                    simulation_cell
                        SC 20.0
                    end
                    cutoff 15.0

                    mult 3

                    xc vosko
                        lmbfgs
                    end


                task pspw energy
```

The pseudopotential block contains parameters that define the calculation.

The simulation cell sub-block defines the parameters of the cell that encloses the system

SC denotes Simple Cubic simulation cell with the length of 20 (in atomic units)

Cutoff energy of the simulation. In this case the cutoff energy is 15au = 30Ry= 408eV

Multiplicity of the system (2s+1). In this case it is triplet.

xc directive specifies VWN local density parametrization of the exchange-correlation functional

Defines a minimization algorithm

Task directive requests the actual calculation. In this case we are using plane wave pseudopotential method (pspw) and requesting total energy calculation.

Much of the content of the output file is self-explanatory. There is a section in the output file that summarizes the setup of the calculation

```
      ....
 s2-pspw-energy.movecs
 -    spin, nalpha, nbeta:            2               7               5

  input psi filename:./perm/s2-pspw-energy.movecs
  Warning - Gram-Schmidt being performed on psi:   12.0000000000000
    7.95390810283378          12.0000000000000          4.04609189716622


  number of processors used:         6
  processor grid           :    6 x   1
  parallel mapping         :    hilbert
  parallel mapping         :   balanced

  options:
       boundary conditions  = periodic    (version3)
       electron spin        = unrestricted
       exchange-correlation = LDA (Vosko et al) parameterization

 elements involved in the cluster:
      1: S     core charge:  6.0000  lmax=  2
            comment    : Hamann pseudopotential
            pseudpotential type              :   0
            highest angular component        :   2
            local potential used             :   2
```

```
          number of non-local projections:    4
          cutoff =    0.843    0.955    0.955


total charge:    0.000

atomic composition:
    S   :  2

number of electrons: spin up=     7 (    7 per task)  down=      5 (    5 per task) (fourier space)
number of orbitals : spin up=     7 (    7 per task)  down=      5 (    5 per task) (fourier space)

supercell:
    cell_name:  cell_default
    lattice:    a1=<  20.000    0.000    0.000 >
                a2=<   0.000   20.000    0.000 >
                a3=<   0.000    0.000   20.000 >
    reciprocal: b1=<   0.314    0.000    0.000 >
                b2=<   0.000    0.314    0.000 >
                b3=<   0.000    0.000    0.314 >
    lattice:    a=       20.000 b=       20.000 c=       20.000
                alpha=  90.000 beta=   90.000 gamma=   90.000
                omega=        8000.0
```

Simulation Cell Parameters

```
    density cutoff= 30.000  fft= 50x 50x 50(     31335 waves     5222 per task)
    wavefnc cutoff= 15.000  fft= 50x 50x 50(     11060 waves     1843 per task)
```

Plane Wave grid information (units for cutoffs are Hartrees)

```
    ewald summation: cut radius=      6.37  and  1
                     madelung= 1.76011888


technical parameters:
    time step=        5.80     ficticious mass=  400000.0
    tolerance=.100E-06 (energy)    0.100E-06 (density)
    maximum iterations =     1000 (    10 inner  100 outer )
```

The calculation results are contained in the `Summary Of Results` section of the output file.

```
==  Summary Of Results  ==

 number of electrons: spin up=    7.00000  down=    5.00000 (real
space)

 total      energy    :  -0.2041357199E+02 (   -0.10207E+02/ion)
 total orbital energy:  -0.4948367461E+01 (   -0.41236E+00/electron)
 hartree    energy    :   0.1683720331E+02 (    0.14031E+01/electron)
 exc-corr   energy    :  -0.4323583819E+01 (   -0.36030E+00/electron)
 ion-ion    energy    :   0.4347470065E-01 (    0.21737E-01/ion)

 kinetic (planewave) :    0.7538857655E+01 (    0.62824E+00/electron)
 V_local (planewave) :   -0.4513502571E+02 (   -0.37613E+01/electron)
 V_nl    (planewave) :    0.4625501881E+01 (    0.38546E+00/electron)
 V_Coul  (planewave) :    0.3367440662E+02 (    0.28062E+01/electron)
 V_xc.   (planewave) :   -0.5652107901E+01 (   -0.47101E+00/electron)
 Virial Coefficient  :   -0.1656381601E+01

 orbital energies:
   -0.1994696E+00 (  -5.428eV)
   -0.1994700E+00 (  -5.428eV)
   -0.3302312E+00 (  -8.986eV)    -0.2999470E+00 (  -8.162eV)
   -0.3302317E+00 (  -8.986eV)    -0.2999484E+00 (  -8.162eV)
   -0.3584029E+00 (  -9.753eV)    -0.3353298E+00 (  -9.125eV)
   -0.5624929E+00 ( -15.306eV)    -0.5238526E+00 ( -14.255eV)
   -0.7658804E+00 ( -20.841eV)    -0.7431111E+00 ( -20.221eV)

 Total PSPW energy   :   -0.2041357199E+02
```

Total Energy Analysis

Energy Levels

Example II: Structural optimization of S2 dimer within LDA approximation

In this example we will optimize the structure of S2 dimer using results generated from prior energy calculation. Since most of the parameters are already stored in the database the input is very simple.

Input file:

```
echo

title "optimization of s2-dimer LDA/30Ry with PSPW method"

restart s2-pspw-energy

scratch_dir ./scratch
permanent_dir ./perm


driver

   maxiter 20

   xyz s2

end


task pspw optimize
```

The "restart" directive indicates that we will reusing the results from our previous calculation. Notice the name of the database file

Previously generated files in permanent directory will be reused

The driver block defines optimization parameters.

Maximum number of iterations is 20

The structural snapshots of the system will be generated at each step in xyz format with file prefix s2 (e.g. s2-001.xyz, …)

Task directive to commence structural optimization using pspw method

As the optimization process consists of series of total energy evaluations the contents of the output file are very much similar to that in Example I. At each step the total energy and force information will be outputed as follows

```
   Step         Energy      Delta E   Gmax     Grms     Xrms     Xmax   Walltime
   ----  ----------------  --------  --------  --------  --------  --------  -------
@    1     -20.41364254  -7.1D-05  0.00004   0.00004   0.00605   0.01048     7.8
```

Step number

Total Energy and its Change with respect to last step

Maximum value of the force and its RMS average

The best way to keep track of the optimization calculation is to run the following command on the output file:

```
grep @  outputfile
```

Example III: Frequency calculation of S2 dimer within LDA approximation

In this example we will calculate the vibrational frequency of S2 dimer for the optimized geometry calculated in Example II.

Input file:

```
echo

title "optimization of s2-dimer LDA/25Ry with PSPW method"

restart s2-pspw-energy

scratch_dir ./scratch
permanent_dir ./perm

freq
 animate
end


task pspw freq
```

The "restart" directive indicates that we will reusing the results from our previous geometry optimization calculation.

Previously generated files in permanent directory will be reused

The frequency block is optional. The animation keyword directs the program to generate XYZ files to animate vibrational modes.

Task directive to commence frequency calculation using pspw method

Output file:

Raw Frequencies including rotational and translation degrees of freedom

....

```
          ----------------------------------------------------
          NORMAL MODE EIGENVECTORS IN CARTESIAN COORDINATES
          ----------------------------------------------------
                (Frequencies expressed in cm-1)

                     1         2         3         4         5         6

Frequency        -70.30    -44.08    -44.08     93.59     93.59    723.42

          1     0.00000   0.12505   0.00000   0.12505   0.00000   0.00000
          2     0.00000   0.00000   0.12505   0.00000   0.12505   0.00000
          3     0.12505   0.00000   0.00000   0.00000   0.00000   0.12505
          4     0.00000   0.12505   0.00000  -0.12505   0.00000   0.00000
          5     0.00000   0.00000   0.12505   0.00000  -0.12505   0.00000
          6     0.12505   0.00000   0.00000   0.00000   0.00000  -0.12505
```

```
 Zero-Point correction to Energy   =      1.034 kcal/mol  (   0.001647 au)
 Thermal correction to Energy      =      2.579 kcal/mol  (   0.004110 au)
 Thermal correction to Enthalpy    =      3.171 kcal/mol  (   0.005054 au)

 Total Entropy                     =     52.277 cal/mol-K
   - Translational                 =     38.368 cal/mol-K (mol. weight =   63.9441)
   - Rotational                    =     13.630 cal/mol-K (symmetry #  =        2)
   - Vibrational                   =      0.279 cal/mol-K

 Cv (constant volume heat capacity) =     5.750 cal/mol-K
   - Translational                 =      2.979 cal/mol-K
   - Rotational                    =      1.986 cal/mol-K
   - Vibrational                   =      0.785 cal/mol-K
```

….

```
          ----------------------------------------------------
          NORMAL MODE EIGENVECTORS IN CARTESIAN COORDINATES
          ----------------------------------------------------
              (Projected Frequencies expressed in cm-1)


                     1          2          3          4          5          6

P.Frequency        0.00       0.00       0.00       0.00       0.00      723.42

           1     0.00000    0.17685    0.00000    0.00000    0.00000    0.00000
           2     0.00000    0.00000    0.17685    0.00000    0.00000    0.00000
           3     0.12505    0.00000    0.00000    0.00000    0.00000    0.12505
           4     0.00000    0.00000    0.00000    0.17685    0.00000    0.00000
           5     0.00000    0.00000    0.00000    0.00000    0.17685    0.00000
           6     0.12505    0.00000    0.00000    0.00000    0.00000   -0.12505
```

The animation frames will saved into your permanent directory. To view the animation corresponding to mode 6 (the true vibrational mode in this particular case) you can concatenate all animation frames into a single file,

```
cat freq.m-006.s-0*xyz > freq.m6.xyz
```

and load it into your favorite visualization program.

Example IV: Molecular dynamics simulation of of S2 dimer within LDA approximation

Input file:

```
echo

title "AIMD simulation of s2-dimer "

start s2-md

scratch_dir ./scratch
permanent_dir ./perm

geometry
S 0.0 0.0 0.0
S 0.0 0.0 1.95
end

nwpw
   simulation_cell
      SC 20.0
   End
   Cutoff 15.0

   mult 3
   xc lda
   lmbfgs
end
```

For the explanation of this portion of the input file see Example I

```
nwpw
  car-parrinello

    time_step 5.0

    fake_mass 600.0

    loop 1  1000

    xyz_filename s2-md.xyz

  end
```

Molecular dynamics step in atomic units

Fictitious mass for the electron degrees of freedom

Number of iterations for inner and outer loops

Name of the XYZ file for trajectory animation

Perform total energy calculation to relax electronic degrees of freedom

end

Commence molecular dynamics simulation with pspw method

task pspw energy

task pspw car-parrinello

Output file:

…..

```
Constant Energy Simulation



       ============ Car-Parrinello iteration ==============
  >>>   ITERATION STARTED AT Mon Aug  9 16:49:05 2010   <<<
 iter.          KE+Energy                Energy          KE_psi           KE_ion   Temperature
 ------------------------------------------------------------------------------------------
    1  -0.2041189672E+02  -0.2041189711E+02   0.99213E-08   0.38229E-06           0.12
    2  -0.2041189672E+02  -0.2041189828E+02   0.29482E-07   0.15244E-05           0.40
    3  -0.2041189672E+02  -0.2041190018E+02   0.46156E-07   0.34130E-05           0.84
    4  -0.2041189672E+02  -0.2041190282E+02   0.67257E-07   0.60281E-05           1.43

  ......
```

Total MD energy   = Total Energy + Electron Kinetic Energy + Ion Kinetic Energy

```
     total      energy   :  -0.2041198722E+02 (   -0.10206E+02/ion)
     total orbital energy:  -0.4973635001E+01 (   -0.41447E+00/electron)
     hartree    energy   :   0.1703713644E+02 (    0.14198E+01/electron)
     exc-corr   energy   :  -0.4342335445E+01 (   -0.36186E+00/electron)
     ion-ion    energy   :   0.2643181903E+00 (    0.13216E+00/ion)

     Kinetic energy (elc)   :    0.4163313222E-05 (    0.34694E-06/elc)
     Kinetic energy (ion)   :    0.8634363416E-04 (    0.43172E-04/ion)

     final kinetic energy:   0.41633E-05 (psi)   0.86344E-04 (ion)
                                                 0.10216E-39 (c.o.m.)
     Temperature :          0.0 K (elc)
     Temperature :        519.3 K (ion)
                 :          0.0 K (c.o.m.)
```