Hands on Session I:

Georg KRESSE

Institut für Materialphysik and Center for Computational Material Science

Universität Wien, Sensengasse 8, A-1090 Wien, Austria

Overview

- discussion of the required files

- lot's of examples

  - O atom

  - O_2 dimer

  - CO

  - H_2O

- tasks

  - relaxation

  - vibrational frequencies

  - MD

The very first step: a single atom

- files required to do all calculations presented in this session can be found in

  ```
  ~vw/1_1_description_of_job1
  ~vw/1_2_description_of_job2
  ```

  first digit corresponds to the number of the hands on session, second one to the example

- required files `INCAR`, `KPOINTS`, `POSCAR`, `POTCAR`

  – `POTCAR` pseudopotential file

   generated by concatenation of individual `POTCAR` files from the data-base

  – `KPOINTS` Brillouin zone sampling

   describes which k-points are used

  – `POSCAR` structural data

   basis vectors and positions

  – `INCAR` steering the calculations

The POTCAR file

- in this course, you can copy the POTCAR files from

  `˜vw/potpaw_PBE/element_name/POTCAR`

  `˜vw/potpaw_PBE/O/POTCAR`

  or simply type

  `makepaw_PBE O`

  or copy all input files from `˜vw/1_1_Oatom`

  `mkdir Oatom ; cd Oatom ; cp ˜vw/1_1_Oatom/* .`

- what information can be found in the POTCAR file:

  - pseudopotential description

  - data that is required to regenerate the potential

  - number of valence electrons

  - atomic mass

  - required energy cutoff

The KPOINTS file

- determines how many k-points are used to sample the Brillouin zone

- for molecules or atoms | only a single k-point is required |

  KPOINTS file:

  ```
  Gamma-point only
   1          ! one k-point
  rec         ! in units of the reciprocal lattice vector
    0 0 0 1  ! 3 coordinates and weight
  ```

- for atoms and molecules the Bloch theorem does not apply, hence there is no need to use more then one single k-point

  when more k-points are used, only the interaction between the atoms (which should be zero) is described more accurately

The POSCAR and INCAR files

- determines the lattice vectors (Bravais lattice) and the coordinates (position of the atoms)

- a single atom POSCAR file:

```
O atom in a box
 1.0               ! universal scaling parameters
 8.0 0.0 0.0  ! lattice vector  a(1)
 0.0 8.0 0.0  ! lattice vector  a(2)
 0.0 0.0 8.0  ! lattice vector  a(3)
1                 ! number of atoms
cart              ! positions in cartesian coordinates
 0 0 0
```

- INCAR steers the calculations:

```
SYSTEM = O atom in a box
ISMEAR = 0
```

Running vasp

type:

```
vasp
 vasp.4.6.2 07Jul02
 POSCAR found :  1 types and      1 ions
 LDA part: xc-table for Pade appr. of Perdew
 POSCAR, INCAR and KPOINTS ok, starting setup
 WARNING: wrap around errors must be expected
 entering main loop
       N       E                dE             d eps   ncg     rms          rms(c)
DAV:   1    0.39156E+02    0.39157E+02   -0.95953E+02   14    0.335E+0
DAV:   2    0.39499E+01   -0.35207E+02   -0.34385E+02   28    0.480E+0
DAV:   3   -0.15830E+00   -0.41082E+01   -0.39042E+01   14    0.376E+0
DAV:   4   -0.31026E+00   -0.15195E+00   -0.13836E+00   14    0.660E+0
DAV:   5   -0.31321E+00   -0.29544E-02   -0.29502E-02   28    0.907E-0   0.286E-01
DAV:   6   -0.31407E+00   -0.86398E-03   -0.18767E-03   14    0.397E-0   0.142E-01
DAV:   7   -0.31422E+00   -0.14198E-03   -0.21862E-04   14    0.149E-0   0.480E-02
DAV:   8   -0.31427E+00   -0.55085E-04   -0.26453E-05   14    0.469E-0
    1 F= -.31427624E+00 E0= -.16001392E+00  d E =-.308525E+00
 writing wavefunctions
```

OSZICAR *and* `stdout` *file*

initial charge corresponds to the charge of isolated overlapping atoms (POTCAR)

for 4 steps the charge remains fixed, then the charge is updated (`rms(c)` column)

`N`	iteration count
`E`	total energy
`dE`	change of total energy
`d eps`	change of the eigenvalues (fixed potential)
`ncg`	number of optimisation steps $\mathbf{H}\psi$
`rms`	total residual vector $\sum_{nk} w_k f_{nk} (\mathbf{H} - \varepsilon_{nk}) \psi_{nk}$
`rms(c)`	charge density residual vector

OUTCAR *file*

individual parts are separated by lines

- first part: reading INCAR, POTCAR, POSCAR

- nearest neighbor distances and analysis of symmetry

- information on what was parsed from INCAR

- verbose job information

- information on lattice, k-points and positions

- information on the basis set (number of plane waves)

- non local pseudopotential information

- information for each electronic step (one line in OSZICAR)

```
POTLOK:  VPU time     0.93: CPU time     0.93
SETDIJ:  VPU time     0.01: CPU time     0.01
EDDAV :  VPU time     0.82: CPU time     0.83
DOS   :  VPU time     0.00: CPU time     0.00
-------------------------------------------
LOOP:  VPU time     1.76: CPU time     1.76


eigenvalue-minimisations  :    14
total energy-change (2. order) : 0.3915659E+02  (-0.9595269E+02)
number of electron    6.0000000 magnetization
augmentation part     6.0000000 magnetization


Free energy of the ion-electron system (eV)
 ---------------------------------------------------------
 alpha Z        PSCENC =          0.27135287
 Ewald energy   TEWEN  =        -91.92708002
 -1/2 Hartree   DENC   =       -281.84385690
 -V(xc)+E(xc)   XCENC  =         26.11949869
 PAW double counting   =        245.99840262      -247.84808825
 entropy T*S    EENTRO =         -0.18330906
 eigenvalues    EBANDS =        -43.69352752
 atomic energy  EATOM  =        432.26319604
 ---------------------------------------------------------
 free energy    TOTEN  =         39.15658846 eV

 energy without entropy =        39.33989752  energy(sigma->0) =       39.24824299
```

- eigenvalues

```
k-point   1 :       0.0000   0.0000   0.0000
  band No.  band energies     occupation
       1     -23.8345     2.00000
       2      -8.8952     1.33333
       3      -8.8952     1.33333
       4      -8.8952     1.33333
       5      -0.4860     0.00000
       6       1.8485     0.00000
       7       1.8486     0.00000
```

- information on charge + some more timing informations

```
 soft charge-density along one line, spin component          1
          0         1         2         3         4         5         6         7         8
 x    5.4925    5.1765    4.3721    3.3741    2.4214    1.6318    1.0341    0.6112    0.3290
```

- information on the energy and stress tensor

```
FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)
-------------------------------------------------------
free  energy   TOTEN  =          -0.314276 eV

energy  without entropy=        -0.005752  energy(sigma->0) =       -0.160014

FORCE on cell =-STRESS in cart. coord.  units (eV/reduce length):
Direction     X         Y         Z        XY        YZ        ZX
----------------------------------------------------------------------------
Alpha Z      0.27      0.27      0.27
Ewald      -30.64    -30.64    -30.64      0.00      0.00      0.00
Hartree     93.89     93.89     93.89      0.00      0.00      0.00
E(xc)      -27.94    -27.94    -27.94      0.00      0.00      0.00
Local     -147.85   -147.85   -147.85      0.00      0.00      0.00
n-local    -20.54    -20.54    -20.54      0.00      0.00      0.00
augment      5.55      5.55      5.55      0.00      0.00      0.00
Kinetic    126.50    126.50    126.50      0.00      0.00      0.00
----------------------------------------------------------------------------
Total       -0.77     -0.77     -0.77      0.00      0.00      0.00
in kB       -2.41     -2.41     -2.41      0.00      0.00      0.00
external pressure =      -2.41 kB  Pullay stress =       0.00 kB
```

- final timing information

Some comments on this particular run

- the relevant energy for molecules and atoms is `energy without entropy`

    ```
    energy  without entropy=  -0.005752  energy(sigma->0) =      -0.160014
    ```

    three degenerate p orbitals are occupied by 2/3 electrons causing a unphysical electronic entropy

    ```
    entropy T*S    EENTRO =        -0.30852464
    ```

- a tiny value for `SIGMA=0.01` would reduce the entropy but might slow convergence (default is `SIGMA=0.2`)

    `SIGMA` controls the electronic temperature, which is not a very meaningful quantity for molecules and atoms

- the total energy is found to be essentially zero

    VASP subtracts from any calculated energy the energy of the atom in the configuration for which the pseudopotential was generated

    all pseudopotentials were generated using non spin polarized reference atoms

Restart vasp in same directory

```
vasp.4.6.2 07Jul02
POSCAR found :  1 types and     1 ions
LDA part: xc-table for Pade appr. of Perdew
found WAVECAR, reading the header
POSCAR, INCAR and KPOINTS ok, starting setup
WARNING: wrap around errors must be expected
the WAVECAR file was read sucessfully
initial charge from wavefunction
entering main loop
      N       E             dE            d eps     ncg     rms       rms(c)
DAV:  1  -0.314277E+00  -0.31428E+00  -0.14320E-06  14  0.899E-03    0.157E-03
DAV:  2  -0.314277E+00   0.64237E-07  -0.19000E-07   7  0.353E-03
   1 F= -.31427731E+00 E0= -.16001499E+00  d E =-.308525E+00
writing wavefunctions
```

when vasp is restarted the WAVECAR file is read and the run is continued from the previous
wavefunctions (converging rapidly)

Spin polarized calculation

- the O atom is an open shell system with **2 unpaired electrons**

- add `ISPIN=2` to the INCAR file remove WAVECAR and restart vasp

  (alternatively copy all input files from~vw/1_2_Oatomspin)

```
vasp.4.6.2 07Jul02
POSCAR found :  1 types and     1 ions
...
entering main loop
       N       E                dE              d eps       ncg       rms          rms(c)
DAV:   1    0.38975372E+02     0.38975E+02    -0.10098E+03    32    0.259E+02
DAV:   2    0.31791299E+01    -0.35796E+02    -0.35789E+02    64    0.438E+01
DAV:   3   -0.11905610E+01    -0.43697E+01    -0.36660E+01    32    0.327E+01
DAV:   4   -0.12616637E+01    -0.71103E-01    -0.69167E-01    32    0.508E+00
DAV:   5   -0.12625234E+01    -0.85968E-03    -0.85961E-03    48    0.504E-01    0.653E+00
...
DAV:  11   -0.16719490E+01     0.16543E-04    -0.47746E-04    32    0.131E-01
   1 F= -.16719490E+01 E0= -.15948179E+01  d E =-.154262E+00  mag=      1.9986
writing wavefunctions
```

Spin polarized calculation

- eigenstates for spin up and spin down are calculated "separately" in LSDA they interact only via the effective local potential spin-up and spin-down potential

- in the OUTCAR file, one can see two spin components

- the spin component 1 has 2 more electrons corresponding the a magnetization of $2\,\mu_B$

```
k-point   1 :        0.0000     0.0000     0.0000
 band No.  band energies     occupation
    1      -25.0761          1.00000
    2      -10.0715          1.00000
    3      -10.0715          1.00000
    4      -10.0715          1.00000
    5       -0.3997          0.00000
    6        1.6965          0.00000
    7        1.9499          0.00000
    8        1.9499          0.00000


spin component 2
k-point   1 :        0.0000     0.0000     0.0000
 band No.  band energies     occupation
    1      -21.8260          1.00000
    2       -7.0425          0.33333
    3       -7.0425          0.33333
    4       -7.0425          0.33333
    5       -0.4479          0.00000
    6        1.9043          0.00000
    7        1.9043          0.00000
    8        1.9043          0.00000
```

Symmetry broken O atom

- in the GGA, most atoms are characterized by a symmetry broken solution

  VASP however symmetrizes the charge-density according to the determined symmetry of the cell

  check the OUTCAR file, which symmetry is VASP using

- to lower the symmetry simply change the lattice parameters to 7.0 8.0 and 9.0 in the POSCAR file (alternatively copy all input files from ˜vw/1_3_Oatomspinlow):

  ```
  7.0 0.0 0.0  ! lattice vector  a(1)
  0.0 7.5 0.0  ! lattice vector  a(2)
  0.0 0.0 8.0  ! lattice vector  a(3)
  ```

  and reduce `SIGMA` to `SIGMA=0.01` (INCAR file)

- rerunning VASP you will find a much lower energy

  ```
  vasp.4.6.2 07Jul02
  ...
  DAV:  17     -0.190131780202E+01   -0.53122E-04   -0.35327E-06    32    0.128E-02
     1 F= -.19013178E+01 E0= -.19013178E+01  d E =-.938468E-52  mag=    1.9997
  ```

Let's add another atom: the O_2 dimer

- copy the required files and start VASP (see footnote)

- POSCAR:

```
O atom in a box
 1.0             ! universal scaling parameters
 8.0 0.0 0.0  ! lattice vector  a(1)
 0.0 8.0 0.0  ! lattice vector  a(2)
 0.0 0.0 8.0  ! lattice vector  a(3)
2               ! number of atoms
cart            ! positions in cartesian coordinates
 0 0 0          ! first atom
 0 0 1.22       ! second atom
```

- INCAR:

```
SYSTEM = O2 dimer in a box
ISMEAR = 0 ! Gaussian smearing
ISPIN  = 2 ! spin polarized calculation
NSW = 5    ! 5 ionic steps
IBRION = 2 ! use the conjugate gradient algorithm
```

Relaxing the O$_2$ dimer

- we have inserted that geometry relaxation should be performed:

  in this case 5 ionic steps (`NSW = 5`) should be done at most

  for the relaxation a conjugate gradient algorithm is used `IBRION = 2`

- CG requires a line minimizations along the search direction
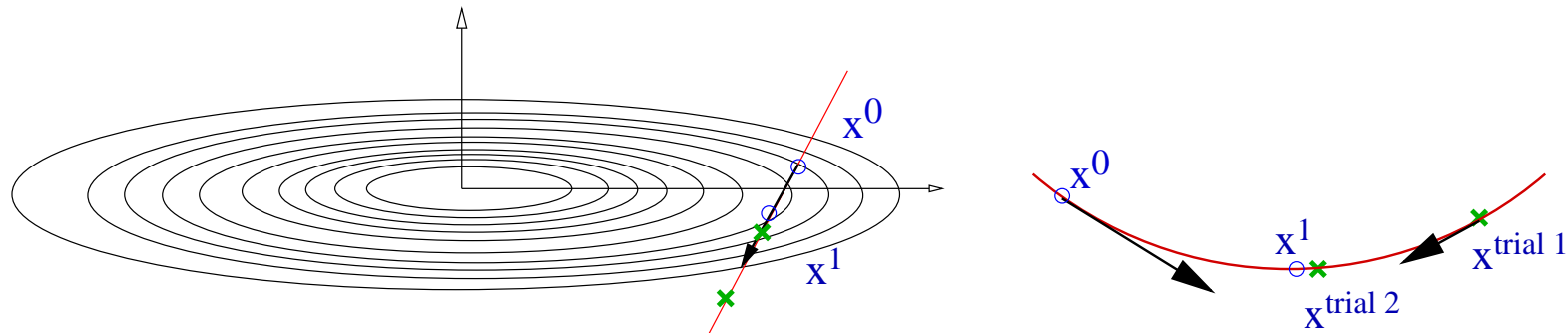
  this is done using a variant of Brent's algorithm

  - trial step along search direction (gradient scaled by `POTIM`)

  - quadratic or cubic interpolation using energies and forces at $\vec{x}_0$ and $\vec{x}_1$ allows to determine the approximate minimum

  - continue minimization, if app. minimum is not accurate enough

Relaxing the O_2 dimer

```
DAV:   1     0.511277926223E+02    0.51128E+02   -0.31305E+03    60   0.528E+02
...
DAV:  11    -0.985454093746E+01   -0.88826E-04   -0.59757E-05    44   0.746E-02
   1 F= -.98545409E+01 E0= -.98545409E+01  d E =-.985454E+01  mag=     2.0000
 curvature:   0.00 expect dE= 0.000E+00 dE for cont linesearch  0.000E+00
 trial: gam= 0.00000 g(F)=  0.111E+00 g(S)=  0.000E+00 ort = 0.000E+00 (trialstep = 0.100E+01)
 search vector abs. value=  0.111E+00
 bond charge predicted

...

   2 F= -.96306943E+01 E0= -.96306943E+01  d E =0.223847E+00  mag=     2.0000
 trial-energy change:    0.223847  1 .order    0.186756   -0.110518    0.484030
 step:   0.1406(harm=  0.1859)  dis= 0.00726  next Energy=    -9.862210 (dE=-0.767E-02)
 bond charge predicted

...

   3 F= -.98624278E+01 E0= -.98624278E+01  d E =-.788682E-02  mag=     2.0000
 curvature:  -0.09 expect dE=-0.448E-05 dE for cont linesearch -0.448E-05
 trial: gam= 0.00000 g(F)=  0.484E-04 g(S)=  0.000E+00 ort =-0.231E-02 (trialstep = 0.828E+00)
 search vector abs. value=  0.484E-04
 reached required accuracy - stopping structural energy minimisation
```

CG: What does all this mean?

- the quantity `trial-energy change` is the change of the energy in the trial step

- the first value after `1.order` is the expected energy change calculated from the forces
  $((\mathbf{F}(\text{start}) + \mathbf{F}(\text{trial}))/2 \times$ change of positions)
  central difference

  second and third value corresponds to $\mathbf{F}(\text{start}) \times$ change of positions and $\mathbf{F}(\text{trial}) \times$ change of positions

- the value `step:` is the estimated size of the step leading to a line minimization along the current search direction

  `harm` is the optimal step using a second order (or harmonic) interpolation

- the trial step size can be controlled by the parameter `POTIM`
  the value `step:` times the present `POTIM` is usually optimal

- the final positions after the optimisation are stored in `CONTCAR`

  you can copy `CONTCAR` to `POSCAR` and continue the relaxation

Let's add another species: the CO molecules

- copy required files and start VASP

- POSCAR:

```
...
1 1           ! number of atoms for each species
cart          ! positions in cartesian coordinates
 0 0 0        ! first atom
 0 0 1.12     ! second atom
```

- POTCAR is created by the concatenation of two individual POTCAR files
  corresponding to O and C; e.g.:

```
cat  ~vw/potpaw_PBE/O/POTCAR  ~vw/potpaw_PBE/C/POTCAR  >POTCAR
```

- a similar relaxation as in the previous case is performed

  but in this case more steps are required, since the first estimate for the minimum is
  not very accurate

  the trial steps are much too long (POTIM parameter)

Relaxing the CO dimer

```
   1 F= -.14764188E+02 E0= -.14764188E+02  d E =-.147642E+02
 curvature:   0.00 expect dE= 0.000E+00 dE for cont linesearch  0.000E+00
 trial: gam= 0.00000 g(F)=  0.822E+00 g(S)=  0.000E+00 ort = 0.000E+00 (trialstep = 0.100E+01)
 search vector abs. value=  0.822E+00
...
   2 F= -.12657048E+02 E0= -.12657048E+02  d E =0.210714E+01
 trial-energy change:    2.107140  1 .order    1.312507   -0.821770    3.446784
 step:   0.1925(harm=  0.1925)  dis= 0.02710  next Energy=   -14.843291 (dE=-0.791E-01)
...
   3 F= -.14747873E+02 E0= -.14747873E+02  d E =0.163154E-01
 curvature:  -0.10 expect dE=-0.909E-01 dE for cont linesearch -0.909E-01
 ZBRENT: interpolating
 opt :   0.0929  next Energy=   -14.802370 (dE=-0.382E-01)
...
   4 F= -.14797047E+02 E0= -.14797047E+02  d E =-.328587E-01
 curvature:  -0.04 expect dE=-0.341E-03 dE for cont linesearch -0.341E-03
 trial: gam= 0.00000 g(F)=  0.844E-02 g(S)=  0.000E+00 ort =-0.833E-01 (trialstep = 0.819E+00)
 search vector abs. value=  0.844E-02
 reached required accuracy - stopping structural energy minimisation
```

Vibrational frequencies of the CO dimer

- ```
  SYSTEM = CO dimer in a box
  ISMEAR = 0    ! Gaussian smearing
  IBRION = 5    ! vibrational spectrum
  NFREE = 2     ! use central differences
  POTIM = 0.02  ! 0.02 stepwidth
  NSW = 1       ! ionic steps must be larger 0 (that's all)
  ```

- POSCAR:

  ```
  sel            ! selective degrees of freedom are changed
  cart           ! positions in cartesian coordinates
   0 0 0      F F T  ! first atom
   0 0 1.143  F F T  ! second atom
  ```

  the selected degrees of freedom are displaced once in the direction $\hat{x}$ and once $-\hat{x}$ by 0.02 Å

  in the present case this makes 4 displacements plus the equilibrium positions (i.e. a total of five ionic configurations)

```
   SECOND DERIVATIVES (NOT SYMMETRIZED)
   --------------------------------------
              1Z          2Z
   1Z  -114.847733   114.847733
   2Z   114.305971  -114.305971


Eigenvectors and eigenvalues of the dynamical matrix
----------------------------------------------------------
   1 f  =    63.876494 THz    401.347846 2PiTHz 2130.690412 cm-1   264.172038 meV
           X          Y          Z          dx         dy          dz
      0.000000   0.000000   0.000000         0          0   -0.655709
      0.000000   0.000000   1.143000         0          0    0.755014
   2 f/i=     0.074763 THz      0.469753 2PiTHz    2.493841 cm-1     0.309197 meV
           X          Y          Z          dx         dy          dz
      0.000000   0.000000   0.000000         0          0   -0.755014
      0.000000   0.000000   1.143000         0          0   -0.655709


Eigenvectors after division by SQRT(mass)
Eigenvectors and eigenvalues of the dynamical matrix
----------------------------------------------------------
   1 f  =    63.876494 THz    401.347846 2PiTHz 2130.690412 cm-1   264.172038 meV
           X          Y          Z          dx         dy          dz
      0.000000   0.000000   0.000000         0          0   -0.163927
      0.000000   0.000000   1.143000         0          0    0.217854
   2 f/i=     0.074763 THz      0.469753 2PiTHz    2.493841 cm-1     0.309197 meV
           X          Y          Z          dx         dy          dz
...
```

H_2O molecules

- POSCAR

```
H2O _2
0.52918    ! scaling parameter
 15 0 0
 0 15 0
 0 0 15
1 2
select
cart
      0.00      0.00      0.00 F F F
      1.10     -1.43      0.00 T T F
      1.10      1.43      0.00 T T F
```

all coordinates are scaled by the factor 0.529

- INCAR:

```
PREC = Normal     ! standard precision
ENMAX = 400       ! cutoff should be set manually
ISMEAR = 0 ; SIGMA = 0.1
IBRION = 1        ! use DIIS algorithm to converge
NFREE = 2         ! 2 independent degrees of freedom
NSW = 10          ! 10 ionic steps
EDIFFG = -0.02    ! forces smaller 0.02 A/eV
```

H_2O molecules: comments

- `PREC = Normal` should be used in vasp.4.6

  sightly more balanced setup than the default `PREC = Medium`

- I strongly urge to set the energy cutoffs manually in the INCAR file , as it gives

  you more control over the calculations

- for the ionic optimisation the DIIS algorithm is used

  this algorithm builds an approximation of the Hessian matrix and converges usually
  faster than the conjugate gradient algorithm

  it is however recommended to set the independent degrees of freedom manually

  `EDIFFG` determines when to terminate relaxation

  positive values: energy change between steps must be less than `EDIFFG`

  negative values: $|\vec{F_i}| < |\texttt{EDIFFG}| \quad \forall i = 1, N_{ions}$

Interpreting the eigenstates of CO

- the `PROCAR` file gives valuable information of the character of the one electron states

  `LORBIT` 10   DOSCAR and l decomposed PROCAR file

  `LORBIT` 11   DOSCAR and lm decomposed PROCAR file

- we use `LORBIT=11` to distinguish p_x and p_z states

- copy the required input files, and check them using an editor

  execute vasp again

PROCAR file:

```
band    3 # energy    -11.46549527 # occ.   2.00000000

ion      s      py      pz      px     dxy     dyz     dz2     dxz     dx2     tot
   1  0.000   0.546   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.546
   2  0.000   0.157   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.157
tot  0.000   0.703   0.000   0.000   0.000   0.000   0.000   0.000   0.000   0.703


band    4 # energy    -11.46549510 # occ.   2.00000000

ion      s      py      pz      px     dxy     dyz     dz2     dxz     dx2     tot
   1  0.000   0.000   0.000   0.546   0.000   0.000   0.000   0.000   0.000   0.546
   2  0.000   0.000   0.000   0.157   0.000   0.000   0.000   0.000   0.000   0.157
tot  0.000   0.000   0.000   0.703   0.000   0.000   0.000   0.000   0.000   0.703


band    5 # energy     -8.76451122 # occ.   2.00000000

ion      s      py      pz      px     dxy     dyz     dz2     dxz     dx2     tot
   1  0.001   0.000   0.135   0.000   0.000   0.000   0.000   0.000   0.000   0.136
   2  0.172   0.000   0.261   0.000   0.000   0.000   0.000   0.000   0.000   0.433
tot  0.173   0.000   0.396   0.000   0.000   0.000   0.000   0.000   0.000   0.569
```

Let's do some a MD for H_2O

- INCAR:

```
PREC = Normal     ! standard precision
ENMAX = 400       ! cutoff should be set manually
ISMEAR = 0 ; SIGMA = 0.1

IBRION = 0        ! molecular dynamics
NSW = 100         ! 100 steps
POTIM = 1.0       ! timestep 1 fs

SMASS = -3        ! micro-canonical ensemble
TEBEG =  2000 ; TEEND = 2000 ! temperature
```

  time step for this system should be around 0.5-0.7 fs

- POSCAR: to save time the box size is reduced to 12 a.u.

- OSZICAR:

```
1 T=   2134. E= -.13655511E+02 F= -.14207209E+02 E0=.. EK= 0.55170E+00 SP= 0.00E+00 SK= 0.00E+00
2 T=   1971. E= -.13643254E+02 F= -.14152912E+02 E0=.. EK= 0.50966E+00 SP= 0.00E+00 SK= 0.00E+00
3 T=   1336. E= -.13629241E+02 F= -.13974630E+02 E0=.. EK= 0.34539E+00 SP= 0.00E+00 SK= 0.00E+00
4 T=   1011. E= -.13624149E+02 F= -.13885486E+02 E0=.. EK= 0.26134E+00 SP= 0.00E+00 SK= 0.00E+00
5 T=   1307. E= -.13629772E+02 F= -.13967549E+02 E0=.. EK= 0.33778E+00 SP= 0.00E+00 SK= 0.00E+00
```

vi
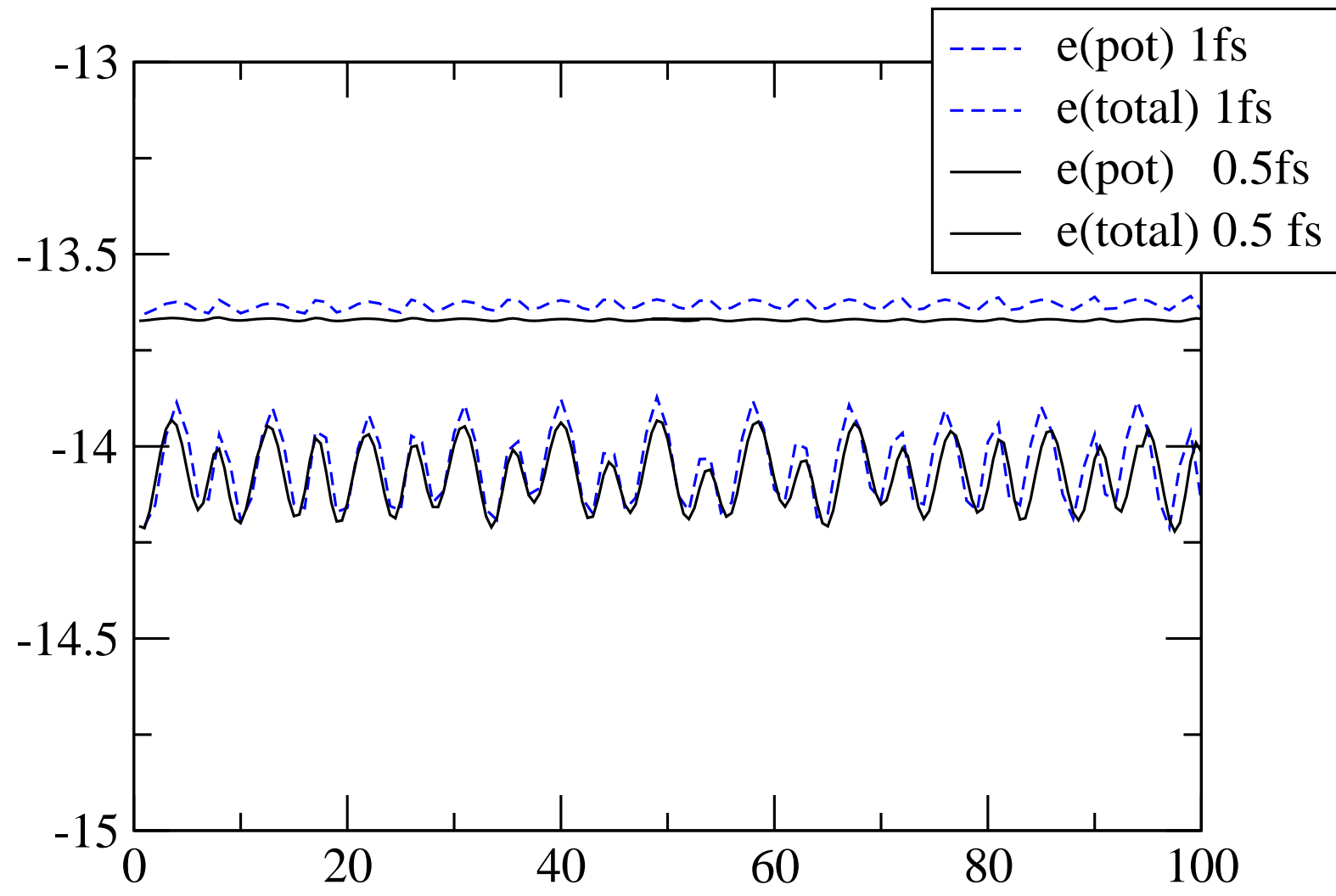
Excersises

- How does the energy change when you decrease `SIGMA` to 0.01 in the INCAR file starting from ˜`vw/1_1_Oatom` ? Why ?

- Try to copy CONTCAR to POSCAR after running the example ˜`vw/1_4_Odimer`. Why is the calculation so fast ?

- Try to play with the parameter `POTIM` for the example ˜`vw/1_4_Odimer`. What is the optimal value ?

- What is the reason for the imaginary frequency in the example ˜`vw/1_6_COvib`. Does the behavior improve when the step width (smaller or larger) is changed. Also try to improve the precession to which the groundstate is converged (`EDIFF=1E-5`). What happens if the accuracy of the calculations is improved (`PREC=Accurate`).

- Try to use the conjugate gradient algorithm to the H_2O molecule (example ˜`vw/1_7_H2O`).

- Calculate the vibrational frequencies of the H_2O molecule (example ˜`vw/1_7_H2O`) after relaxation (example ˜`vw/1_8_H2Ovib`). Why does one find 3 modes that have

small frequencies. `EDIFF=1E-5` gives much improved results than `EDIFF=1E-4`, can you reproduce this behavior.

The following participants have to share one terminal:

Müller and Sahli (ETH Zürich)

Koza and Poehlmann (Univ. Montpellier)

Mok and Soon (Univ. Singapore)

Calatyyud and Mguig (Univ. P.and M. Curie)

possibly, if we encounter troubles:

Hobbs and Milazzo (Kings College, London)

Garcia-Vergniory and Rodriguez (Univ. Bilbao, Spain)

Cordente and Ricardo Chavez (Univ. Toulouse)