MOLECULAR DYNAMICS IN VASP (HOW TO)

Required files: standard INCAR, POSCAR, POTCAR and KPOINTS

Initial velocities (vx, vy, vz) can be specified in the POSCAR file after the coordinate block (cx, cy, cz) as follow (units Å/fs):

```
cx1 cy1 cz1 T T T
cx2 cy2 cy2 T T T
...
cxn cyn czn T T T

vx1 vy1 vz1
vx2 vy2 vy2
...
vxn vyn vzn
```

If initial velocities are not specified, an initial Boltzmann distribution is assumed for the corresponding simulation temperature given in the INCAR file (TEBEG/TEEND). Initial velocities explicitly given in the POSCAR file **prevail** over specified TEBEG and TEEND keywords in the INCAR file. In order to continue a simulation it is only necessary to copy CONTCAR to POSCAR file and restart VASP, since after each ionic iteration the CONTCAR file is updated with both new coordinates and velocities.

A standard INCAR file to perform a NVE MD calculation reads:

```
## PREC = Low       ! Standard precision
ENMAX    = 600.0    ! Cut-off energy
ISMEAR   = 0        ! Partial occupancies scheme: 0 Gaussian smearing
SIGMA    = 0.1      ! Width of the smearing in eV
EDIFF    = 1E-7     ! Allowed error in total energy
LREAL    = .FALSE.  ! Real space projections
NELMIN   = 4        ! Minimum SCF electronic cycles per step
IBRION   = 0        ! It sets molecular dynamics calculation
NSW      = 800      ! Number of molecular dynamics steps
##NBLOCK  = 100     ! How often kinetic energy is scaled (in # of steps)
POTIM    = 1        ! Time step in fs
MAXMIX   = 45       ! Maximum number steps stored in Broyden mixer scheme
SMASS    = -3       ! Nose Hoover mass: -1 Scaled-NVE; -3 free-NVE
TEBEG    = 1000     ! Initial temperature
TEEND    = 1000     ! Final temperature
```

Few considerations should be taken into account to avoid a spurious drift of the total energy of the system along the simulation time (NVE, SMASS=-3; NVT, SMASS=0):

1. **Initial stabilization of the system**. Prior to production, it is highly desirable to stabilize the system, since typically huge initial oscillations of both total energy and temperature are observed, resulting in possible deviations from the desired initial geometries/conditions. To this end it is convenient to scale the kinetic energy (SMASS=-1) after a given number of steps (NBLOCK). A possible working scheme reads: (i) after choosing the initial (working) temperature (TEBEG=TEEND=T_w) one sets NSW=1000 and NBLOCK=5 in the INCAR file; (ii)

The CONTCAR file obtained is then used as input for a new simulation where now one should increase NBLOCK to 25; (iii) this process can be repeated increasing gradually NBLOCK. Before increasing NBLOCK after each scaling block, the total energy and temperature should oscillate in a reasonable range and be as constant as possible; if this is not the case, one can restart the simulation keeping the same NBLOCK. This scheme is quite subjective and the performance depends on the given system. Typically a series of NBLOCK =5/25/100/200 simulations with 1-2 ps per block should be enough to start production. For the productive simulation (free NVE), NBLOCK keyword should be commented.

2. **How to avoid total energy drifting**. The INCAR file above is already a highly robust setup in order to avoid energy drifting problems. The main keywords one should take care of are: PREC, ENMAX, EDIFF, NELMIN, POTIM and MAXMIX. In principle PREC=Low should provide a good compromise accuracy/performance, but some times this setting can not be enough and one should increase manually the cut-off energy by means of ENMAX, which results of course in an increase of the computational cost. Another source of energy drifting concerns the accuracy of the SCF cycles at each ionic step (EDIFF); normal accuracy use to be not enough and a save setting is EDIFF = 1E-7. An alternative way to control this issue is using NELMIN (minimum number of SCF cycles performed at each step) instead of EDIFF or in combination. The time step (POTIM) should be chosen carefully; small values improve the drifting, but increase the total simulation time dramatically. MAXMIX defines the mixing percentage between the old electron density of the previous step and the new one, which impacts on the convergence and, therefore, in the performance. It is worth playing with all this parameters in order to get the best accuracy/performance compromise.

Analysis of the data

The evolution of the energy and temperature of a MD simulation are printed in the OSZICAR file after each electronic SCF:

T: corresponds to the current temperature.
E: total free energy (including the kinetic energy of the ions and the energy of the Nosé thermostat). **This energy should be constant in a proper NVE/NVT simulation** (small drifting).
F: total free energy.
E0: total free energy for *sigma* $\rightarrow 0$.
EK: kinetic energy.
SP: potential energy of the Nosé thermostat.
SK: kinetic energy of the Nosé thermostat.

The program `vaspmd.pl` helps to quickly analyze all this data. It generates several free format files that can be used directly as input to standard graphical utilities and a `movie.xyz` file with the atomic evolution of the system along the simulation. The most important of those files is `vaspmd.E.out`, which contains 5 columns: (i) time in ps, (ii) E, (iii) F, (iv) EK and (v) T. Input files for Gnuplot (`*.gpt`) are automatically generated as well, allowing a quick plotting of the main quantities by simply typing in the prompt:

```
gnuplot -persist vaspmd.E.gpt
```

The program `vaspmd.pl` can be executed as follows:

```
perl vaspmd.pl vaspmd.dat
```

where the `vaspmd.dat` file contains the paths and names of the OSZICAR and OUTCAR files to be processed and concatenated (if more than one single string) in the given order (without **any blank line** at the end):

```
1 0
./PATH_RUN_1/OSZICAR ./PATH_RUN_1/OUTCAR
./PATH_RUN_2/OSZICAR ./PATH_RUN_2/OUTCAR
./PATH_RUN_3/OSZICAR ./PATH_RUN_3/OUTCAR
...
```

The first number in the first line corresponds to the time step (`POTIM`). The second number specifies how many distances between atoms are going to be analyzed (outputs `vaspmd.G.out` and `vaspmd.D.out`), if any. If this number is larger than 0 then the distances of interest are defined as in the example below:

```
1 3
3 4
4 5
6 7
./PATH_RUN_1/OSZICAR ./PATH_RUN_1/OUTCAR
./PATH_RUN_2/OSZICAR ./PATH_RUN_2/OUTCAR
./PATH_RUN_3/OSZICAR ./PATH_RUN_3/OUTCAR
```

where, in this case, the time evolution of distances between atoms 3 and 4, 4 and 5, and 6 and 7 (numbers determined by the order specified in the POSCAR file) will be computed.