4.1 Input files

The TBMD program requires the following input files to run : `INTBMD`, `POSTBMD` and `TBPARAM`.

`INTBMD` : This is the input file that is used to specifies the type of the calculation. The format of the file is free, it consists of of a list of commands in the form `key_word = value(s)`. You can have more than one command per line separated by a semi-column. Here is an example :

```
!  Example INTBMD for FCC Cu
system_name = "Cu fcc unitcell"
dt = 0.3 !  time step for MD
ionic_eom_algo = 1
elec_algo_gs = 2 ; elec_algo_md = 2
number_of_ionic_steps = 1000
ionic_thermostat = .TRUE.
q_nose_ions = 500.0
temperature = 75.0
```

Most of the keywords are self-explanatory but here is a list describing the most important ones :

`system_name` : String that will appear at the top of the main output file.

`ionic_algo` : Algorithm used to move the ions : 0 for molecular dynamics, 1 for conjugate-gradient relaxation and 3 simple steepest-descent relaxation (this is MD with velocities put to zero at each step).

`number_of_ionic_steps` : Number of ionic steps (!), this can be MD or relaxation steps. Default = 0 (i.e. the ions remain fixed).

`mass` : Specify the mass of the ions. The default value is taken from the parameter file `TBPARAM`. Should be given in atomic mass units.

`mu` : Fictitious mass of the electrons. Default is 0.01×`mass`.

`dt` : Time step used for integrating the equations of motion of the system. Given in fs. Default is 0.01 fs for fictitious dynamics and 1 fs otherwise.

`calc_forces` Indicates if forces should be calculated. Default is `.TRUE.`

`ionic_thermostat` : Possible values : `.TRUE.` or `.FALSE.`. Indicates if a Nosé thermostat should be used for the ions when doing molecular dynamics. The temperature of the system will fluctuate around the value given by `'temperature'`. For large enough systems and an appropriate choice of the mass of the thermostat Q_i the MD will sample the canonical ensemble. Default is `.FALSE.`.

`temperature` : Temperature of system.

`q_nose_ions` : Mass associated with the Nosé thermostat for the ions.

`electronic_thermostat` : Possible values : `.TRUE.` or `.FALSE.`. Indicates if a Nosé thermotstat should be used for the electrons when doing fictitious dynamics. The fictitious kinetic energy of the electrons $E_{e,kin}$ will fluctuate around the value given by `'e_kin_elec_target'`. Default is `.FALSE.`.

`e_kin_elec_target` : Target value for $E_{e,kin}$

`q_nose_elec` : Mass associated with the Nosé thermostat for the electrons.

`ionic_friction` : Friction coefficient used to damp the motion of the ions. WARNING : not implemented with fictitious dynamics yet. Default is 0.0.

`pos_input` Give an alternative name to the position file, default is `POSTBMD`.

`status_output_freq` : Frequency at which the system status is written to the output file. Default is 1.

`output_level` : Controls the amount of output. Default is 1.

`'r_cut'` Cut-off radius used to defined nearest-neighbor list. Default is taken from the parameter file `TBPARAM`.

`ionic_eom_algo` : Algorithm used to integrate the ionic equations of motions. Possible values : 1 for Verlet algorithm and 2 for velocity-Verlet. Default is 1.

`elec_gs_algo` : Algorithm used to find the initial ground state. Possible values : 1 for conjugate-gradient minimization, 2 for diagonlization. Default is 2.

`elec_md_algo` : Algorithm used to keep the electrons in the ground state initial ground state. Possible values : 0 for fictitious dynamics, 1 for conjugate-gradient minimization, 2 for diagonlization. Default is the value of `elec_gs_algo`.

`elec_energy_tol` L: Precision to which the minimization of the electronic energy will be done. Default = 10^{-6}.

`max_elec_iter` Maximum number of electronic iterations. Default = 10000.

`min_elec_iter` Minimum number of electronic iterations. Default = 3.

`start` : Restart the calculation. Possible values : 0 start from scratch, 1 will read the initial wave-function from `WFTBMD`. Default is 0.

`eta` Starting value of the η parameter used in unconstrained minimization. WARNING : make sure to use a large enough value, if too small the unconstrained minimization will give unpredictable results. The default of 50.0 was found to be large enough for most cases. The value of η is adjusted during the minimization (see next few keyword) to accelerate convergence. This is a trial and error procedure, it is not always stable, if problems occur set `eta_mod_freq` to a large value in order to keep fixed.

`eta_mod_freq` : The unconstrained minimization parameter η will be adjusted every `eta_mod_freq` CG steps. Default is 10.

`eta_mod_delay` : Number of CG steps done before attempting to change η. Default is 5.

`eta_mod_frac` : Fraction by which η is changed, default is 0.8.

`eta_mod_fail_max` : Maximum number of failures allowed for changing η, when this number is reached η will not be adjusted anymore.

POSTBMD : File containing the description of the unitcell/supercell and the positions and velocities of the atoms. Format is free. Here are two examples :

```
!  POSTBMD for FCC Cu
a0 = 3.61
a_1 = 0.0 0.5 0.5
a_2 = 0.5 0.0 0.5
a_3 = 0.5 0.5 0.5
unit_cell_grid = 6 6 5
number_of_basis_ions = 1
Positions = Unit
0.0 0.0 0.0
```

```
!  POSTBMD for Cu4 cluster
a0 = 12.0
a_1 = 1.0 0.0 0.0
a_2 = 0.0 1.0 0.0
a_3 = 0.0 0.0 1.0
number_of_ions = 4
Positions = Unit
0.0 0.0 0.0
Positions = Cartesian
0.0 0.0 0.0
2.8 0.0 0.0
0.0 2.5 0.0
1.5 1.2 1.0
Velocities = Unit
-5.19016e-05 5.88313e-06 -2.75206e-05
-5.44472e-06 -1.45381e-05 -2.72095e-05
1.42977e-05 -9.61665e-06 -1.92899e-05
-4.97803e-06 3.46058e-05 -3.38563e-05
```

Here is a list describing the keyword found in the `POSTBMD` file :

`a_1`, `a_2` and `a_3` : Lattice parameters.

`a0` Lattice constant which will multiply the lattice parameters.

`number_of_basis_ions` : Number of basis ions in the unit cell. The basis ions will be used to generate a super-cell (see `unit_cell_grid` below).

`number_of_ions` : Number of ions in the super-cell.

`unit_cell_grid` : Three integers (N_x, N_y, N_z) used to generate a super-cell by repeating the unit-cell N_x times along a_1, N_y times along a_2 and N_z times along a_3. This is only used if `number_of_basis_ions` is specified.

`positions`: Indicates if the positions of the ions are given in units of the lattice constants (`Unitcell`) or in Cartesian coordinates (`Cartesian`). This line should be immediately followed by the ionic coordinates.

`velocities`: Same as for `positions` for the velocities. This part is optional.

TBPARAM : Contains information about element and the parameters of the TB model. Except for the 4 lines header this file is identical to the parameter files you can get from the NRL WWW page (`http://cst-www.nrl.navy.mil/bind/`) or generated by the parameter fitting program. If you get/generate a new parameters file you will have to add the header by hand as in the following example for Carbon :

```
NN
Carbon
12.01
2.0 2.0 0.0
4 10.5 0.5
.126103109130E+01   0  1   lambda          (equation 7)   Carbon
-.131170133887E+00  0  2   a_s             (equation 9)   (sp basis)
.180775174776E+01   0  3   b_s             (equation 9)   R_cut = 10.5
                    ⋮
.000000000000E+00   1  95  f_dd delta      (equation 11)  (Overlap)
.000000000000E+00   1  96  fbar_dd delta  (equation 11)  (Overlap)
.100000000000E+01   1  97  g_dd delta      (equation 11)  (Overlap)
```

The first line should start with NN, this is a format descriptor. The second line is a string that indicates for which element the parameters are for, it will be printed to the ouput. The third lines describes the "electronic-structure" of the element in the form : number of s electrons, number of p electrons and number of d electrons. This is used to set the number of electrons per atom and calculate the number of states. The fourth line gives the number of atomic orbitals used (4 for sp elements and 9 for spd), the R_{cut} and the l_0 parameters of the NRL NO-TB model. The rest of the files contains the parameters of the model, only the first column is read.

4.2 Output files

OUTTBMD : Output file.

POS : File in which the positions of the ions are saved every `status_output_freq` MD steps.

ENE : Contains several energies to monitor the MD run. The different energies are indicated at the top of the file. These are different depending on whether fictitious Lagrangian or ordinary MD is done.

EIG.OUT : Eigenvalues if available.

ERRTBMD : File containing possible error and/or warning messages.

POSTBMD.OUT : File containing positions and velocities of the atoms for the last configuration. Used to continue a calculation.

WFTBMD.OUT : File containing the c_α^i for the last configuration. Used to continue a calculation.