Manual

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The main input file contains all of the options for running the program. The name of the file is passed to the program through the command line (if no file name is passed, the default input file is dynamics.in). The file is separated into sections:

Section $method contains paths to the driver programs for running the calculations.

$method

qm — **No default.**
Path to driver for QM calculation.

mm — **No default.**
Path to driver for MM calculation.

overlap — **Required.**
Path to program for calculating wave function overlaps. Required when nonadiabatic coupling vectors are not available.

Section $system contains information about the number of states and initial state of the system.

$system

nstate # — **No default.**
Number of states in the QM system. Required input.

istate # — **nstate**
Initially populated state.

geometry — **geom**
File containing the masses and initial positions of the atoms.

velocity — **veloc**
File containing the initial velocities of the atoms.

Section $output contains options for program output and backup.

$output

outfile — **dynamics.out**
Name of the main output file.

(no)print — **1-7, 9, 10**
Select which variables to print to the main output file.

- 1 - Current electronic state.
- 2 - Coordinates.
- 3 - Velocities.
- 4 - Gradients.
- 5 - Energies. Format:
  Total, Potential, Kinetic.
  QM Potential, QM Kinetic
  MM Potential, MM Kinetic
- 6 - QM state energies.
- 7 - Total electronic wave function coefficients.
- 8 - Coupling mask (logical array determining which couplings will be calculated in current step.)
- 9 - Overlap matrix.
- 10 - Coupling matrix.
- 11 - QM oscillator strengths.

bufile — **backup.dat**
Name of backup file.

buinterval # — **1**
The backup file is written every # steps.

Section $dynamics contains options for the propagation of the nuclear coordinates.

$dynamics

nstep # — **10**
Maximum number of steps for the propagation of nuclear coordinates.

tstep # — **0.5**
Time step for the propagation of nuclear coordinates. Input should be in femtoseconds.

orient (on/off) — **off**
Keeps the molecule in the Eckart frame during the dynamics.

Section $surfhop contains options for the surface hopping procedure and the propagation of the electronic wave function.

$surfhop

tdse_steps # **10000**

Number of substeps for electronic wave function propagation. Hopping probabilities are calculated at each substep. Energies and couplings are linearly interpolated between the nuclear steps.

decoherence **nldm**

Method used for applying a decoherence correction to the electronic wave function. Possible options:

- [off] No decoherence correction.
- [nldm] Granucci/Persico algorithm suggested in J. Chem. Phys. 126 (2007) 134114.

coupling **overlap**

Method used for calculating the coupling matrix. Possible options:

- [nadvec] Calculated from analytic nonadiabatic coupling vectors.
- [overlap] Calculated using the finite difference method from the overlap matrix between the electronic wave functions in the previous and current step.

skip_state **none**

Give list of electronic states which will not be included in the calculation of the couplings. (Example: skip_state 1-2, 5)

reduce_cmat **0**

Reduce the number of coupling matrix elements calculated during each step. Possible options:

- [1 #] Only # states around the current state are included.
- [2 #] Only states in a # eV energy window of the current state are included.
- [3 #] Couplings between each state and # states around it are calculated.
- [4 #] Couplings between each state and states in a # eV energy window around it are calculated.

seed # **-1**

Give a seed for the random number generator. If no seed is given, or seed is ¡= 0, a seed is generated automatically based on the current time and job ID.

A stopped or finished trajectory can be restarted by adding the $restart keyword to the input file. In this case, the backup file is read before restarting the calculation.

In addition to the main input file, the program needs the geometry and velocity file containing the initial conditions for the dynamics run. By default these are called "geom" and "veloc". The geometry file contains a line of six columns for each atom: atom symbol, atom mass, x, y, z, q/m. The final column should be either "q" (for QM) or "m" (for MM). The velocity file contains just the initial velocity vector for each atom.