Documentation - MD_Evaluation

Program to evaluate MD output files of bulk simulations
Notes:

- usable for LAMMPS simulations in metal units
- required files provided by specific LAMMPS scripts

1. Overview

Programm evaluates three different simulation types:

- Evaluation of **single run simulations** for transport properties (**single_run**)
- **Time decomposition method (TDM)** for transport properties (**tdm**)
- Evaluation of **VLE simulations** (two phase simualtions) (**vle**)

Single run simulations

Required Folder structure:

- *SIM_1* [contains all output files of a EMD simulation of one state point]
- …

TDM

Required Folder structure:

- *STATE_1* [contains all simulations of one state point]
  - *Sim_001*
  - *Sim_002*
  - …
- …

VLE simulations

Required Folder structure:

- *FOLDER_1* [contains all simulations done for one substance]
  - *Sim_T1* [VLE simulation at temperature T1]
  - *Sim_T2* [VLE simulation at temperature T2]
  - …
- …

2. Input File

Name: 'INPUT.txt' (has to be in same folder as 'Master' file)

General structure:

- first line: '#' + 'keyword'
- second line: value assigned to keyword

Keywords:

Name	Type {*standard value*}	Modes	Description
mode	string [*single_run*, *tdm*, *vle*]	all	defines the mode of the simulations/evaluation
folder	string	all	path to main folder containing all simulation data (see chapter 1)
ensemble	string [*NVT*, *NVE*, *NpT*]	single_run, tdm	ensemble to evaluate
timesteps_EQU	interger (≥ 0)	all	number of timesteps to ignore at the start of each simulation
DO_single	integer [0,1]	tdm	1 - evaluate single folders, 0 - single folders already evaluated
DO_state	integer [0,1]	tdm	1 - evaluate complete thermodynamic state (main folder)
N_boot	integer (≥ 0)	tdm	number of bootstrapping repetitions
corr_length	integer (≥ 0)	single_run	length (timesteps) of correlation function
span_corr_fun	integer (≥ 0)	single_run	timesteps between single correlation functions
DO_structure	integer [0,1] {*0*}	all	1 - do structure evaluation, 0 - skip structure evaluation
N_bin	integer (≥ 0) {*100*}	all	number of bins for rdf calculation
r_cut	float (unit: Å) {*10 Å*}	all	cut-off radius for rdf calculation
units	string [*real*, *reduced*] {*real*}	all	units of simulation (real: LAMMPS SI units, reduced: reduced by LJ parameters)

Example *single*:

```
# Mode
mode          =   single_run

# Folder
folder        =   C:/path2simulations/sim_1
folder        =   C:/path2simulations/sim_*

# Ensemble and equilibration
ensemble      =   NVT
timesteps_EQU =   0

# Settings for acf
corr_length   =   100000
span_corr_fun =   20000
```

Example *TDM*:

```
# Mode
mode          =   tdm

# Folder
folder        =   C:/path2simulations/sim_1
folder        =   C:/path2simulations/sim_*

# Ensemble and equilibration
ensemble      =   NVT
timesteps_EQU =   0

# TDM Settings
```

```
DO_single     =   1
DO_state      =   1
N_boot        =   100
```

Output

Units:

- Length: [L] = m
- Mass: [m] = g/mol
- Time: [t] = s
- Temperature: [T] = K
- Pressure: [p] = MPa
- Density: [ρ] = g/ml
- Energy: [E] = eV
- Viscosity: [η] = Pa*s
- Diffusion Coefficient: [D] = m²/s
- Thermal Conductivity: [λ] = W/(m*K)