MD - Bulk Evaluation

Program to evaluate MD output files of bulk simulations
Notes:

- usable for LAMMPS simulations in metal units
- required files provided by LAMMPS scipt "in.output"

Manual

Required Folder structure:

- "STATE_1"
  - "Sim_001"
  - "Sim_002"
  - …
- "STATE_1"
  - "Sim_001"
  - "Sim_002"
  - …
- …

Input File

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

Format:

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

Keywords:

Name	Type	Description
modus	string ["transport","vle"]	defines the present simulation as 'transport' or 'vle' Simulations
folder	string	path to main folder containing all simulation data of one thermodynamic state (can occur multiple times), asterisk at the end → all folders one level below are evaluated
ensemble	string ["NVT","NVE","NpT"]	ensemble to evaluate
timesteps_EQU	interger (≥ 0)	number of timesteps to ignore at the start of each simulation
DO_evalulation	integer [0,1]	1 - evaluate single folders, 0 - single folders already evaluated
DO_state	integer [0,1]	1 - evaluate complete thermodynamic state (main folder)
N_boot	integer (≈ No. simulations)	number of bootstrapping repetitions

Example:

> #folder
>
> F:/MD_Bulk/Others/Methane/2020-04-16_trappe-ua/SIM_T_273.15K_rho_0.1gml
>
> #folder
>
> F:/MD_Bulk/Others/Methane/2020-04-16_trappe-ua/*
>
> #ensemble
>
> NVT
>
> #timesteps_EQU
>
> 0
>
> #DO_evaluation
>
> 1
>
> #DO_state
>
> 1
>
> #N_boot
>
> 5

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)