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
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)