MedeA: Surface Tension: Ease the Tension in Surface/Interfacial Tension Calculations

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1 Introduction

MedeA Surface Tension computes the surface and interfacial tension of a range of liquids, molten materials, and interfaces. The module performs molecular dynamics using *MedeA LAMMPS* to evaluate the difference between the time averaged stress tensor components perpendicular and tangential to the interface direction defined by the xy-plane of the input slab model.

$$\gamma_{av} = \frac{L_z}{2}[\langle P_{zz}\rangle - \frac{1}{2}(\langle P_{xx}\rangle + \langle P_{yy}\rangle)] \quad (1)$$

Key Benefits

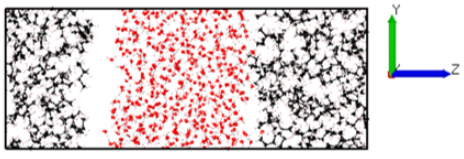
- Automated setup, execution, and analysis of LAMMPS molecular dynamics simulations for surface and interfacial tension calculations
- Handles model construction and assignment of forcefield atom types and charges in one unified environment so that there is no need to use external tools
- Performs analysis of surface/interfacial tension with graphs showing convergence for a given simulation

Hint: The *MedeA Surface Tension* module works with molecular dynamics simulations using LAMMPS. Ab initio MD trajectories are not currently supported with the *Surface Tension* module.

2 *Surface Tension* Usage

The **Surface Tension** stage computes the stress tensor components during a molecular dynamics simulation in the canonical (NVT) ensemble.

To start with, your fluid model must be a slab model with interface planes perpendicular to the z-axis, and appropriate forcefield parameters assigned to all atoms:

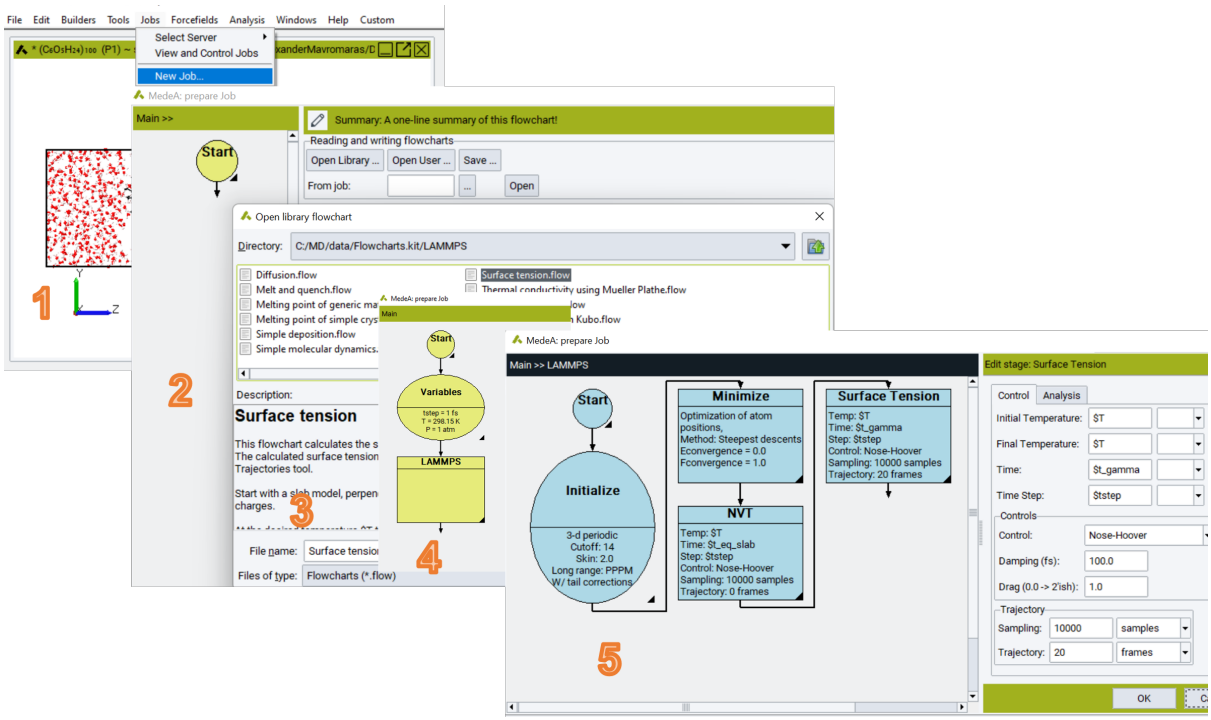


Atoms

Y	Z	Freeze	Occupancy	Spin	FF Atom Type	FF Charge
0.440562	0.570188	---	1	0	o*	-0.806
0.458511	0.583773	---	1	0	hw	0.403
0.464172	0.56256	---	1	0	hw	0.403
0.455429	0.610673	---	1	0	o*	-0.806
0.476959	0.620932	---	1	0	hw	0.403
0.450629	0.618252	---	1	0	hw	0.403
0.871353	0.621564	---	1	0	o*	-0.806

You can insert the **Surface Tension** stage into any *MedeA LAMMPS* Flowchart. To get started quickly, load a template *Surface Tension* workflow from the *MedeA* Flowchart library:

- Click on the structure window containing your fluid system and select New Job... from the Jobs menu.
- In the Flowchart editor window that appears, click Open library... and select the file *Surface tension.flow* from the LAMMPS directory.



The *Surface Tension* workflow has one **LAMMPS** stage with four substages, namely **Initialize** to set some input parameters, **Minimize** to relax the system with fixed cell parameters, **NVT** to equilibrate, and **Surface Tension**, the production run, also in the NVT ensemble, to evaluate the stress tensor components. You can inspect and modify this Flowchart to fit your system and computational goals. Double-click the **LAMMPS** stage to see these substages. Double-click any substage to inspect and edit paramers. The parameters of the **Surface Tension** stage are:

- *Initial Temperature*: The initial temperature setpoint for the thermostat.
- *Final Temperature*: The final temperature setpoint for the thermostat.
- *Time*: The amount of time to use for the surface tension calculation.
- *Time Step*: The time step size employed in solving the equations of motion.
- *Control*: The thermostat algorithm to be used for the NVT ensemble.
- *Sampling*: The quantity of samples, steps, or time to use for gathering statistics.
- *Trajectory*: The quantity of frames, steps, or time that defines how often configurations are written to a trajectory file.

3 *Surface Tension* Output

After completing a *Surface Tension* simulation, results are written to *Job.out* and a plot of the surface tension evolution during the production run is stored in a stage subdirectory on the JobServer. The *MedeA Surface Tension* template Flowchart creates *gif* and *png* output, e.g., *<Job_number>/Stage 2/2.7_surface_tension.png*.

Stage 2.7: Surface tension calculation using NVT integration
for 200 ps with a timestep of 1 fs, T is 298.15 K

Property	Value	+/- Uncertainty	Units	After Steps	% Run
t:	200000		fs		
T:	298.135	+/- 0.026	K	0	0.0%
P:	-62	+/- 26	atm	0	0.0%
V:	38456.4	+/- 7.8e-10	Ang^3	0	0.0%
rho:	0.761066	+/- 0	g/mL	0	0.0%
Etotal:	-7165	+/- 32	kJ/mol	0	0.0%
Epot:	-18316	+/- 32	kJ/mol	0	0.0%
Ekin:	11151.06	+/- 0.96	kJ/mol	0	0.0%
Evdw:	1350	+/- 34	kJ/mol	0	0.0%
Ecoul:	-21160	+/- 69	kJ/mol	0	0.0%
Sxx:	109	+/- 26	atm	0	0.0%
Syy:	87	+/- 33	atm	0	0.0%
Szz:	-11	+/- 25	atm	0	0.0%
Syz:	2	+/- 8.2	atm	0	0.0%
Sxz:	-2	+/- 11	atm	0	0.0%
Sxy:	6	+/- 16	atm	0	0.0%
Surface_Tension:	35.9	+/- 5.2	mN/m	0	0.0%