

# 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.

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

#### **Key Benefits**

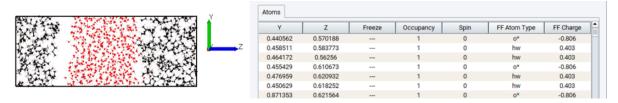
- Automated setup, execution, and analysis of LAMMPS molecular dynamics simulations for surface and interfacial tension calculations
- Handles model construction and assignment of forcefield atom types and charges in one unified environment so that there is no need to use external tools
- Performs analysis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





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			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%

#### Surface Tension versus Time

