

LJ units conversion: <http://lammps.sandia.gov/doc/units.html>

1 Temperature (LJ) Computation

Formula:

$$k_e = \frac{3}{2} N k_b T \quad \text{http://lammps.sandia.gov/doc/compute_temp.html}$$

$$k_e = \frac{3}{2} \sum_{i=1}^N m_i v_i^2$$

Then, one obtains

$$T = \frac{\sum_{i=1}^N m_i v_i^2}{3Nk_b} \Rightarrow T = \frac{\sum_{i=1}^N m_i v_i^2}{3(N-1)k_b} \quad (\text{since command "velocity" force linear moment to be zero, so } N \text{ should minor one DOF.})$$

See, <http://lammps.sandia.gov/doc/velocity.html>

Cited from website link above: *The option defaults are dist = uniform, sum = no, **mom = yes**, rot = no, temp = full style on group-ID, loop = all, and units = lattice.*

Dimensionless form derivation:

$$T^* = \frac{T k_b}{\epsilon} \Rightarrow T = \frac{T^* \epsilon}{k_b}$$

$$v^* = v \sqrt{\frac{m \sigma^2}{\epsilon}} \Rightarrow v = v^* \frac{\sigma}{\sqrt{\frac{m \sigma^2}{\epsilon}}} = v^* \sqrt{\frac{\epsilon}{m}}$$

Finally, the dimensionless formula for temperature computation could be written as follow,

$$T^* = \frac{\sum_{i=1}^N v_i^{*2}}{3(N-1)} \quad (\text{Indeed, Temperature fits perfectly well!})$$

2 Pressure (LJ unit)

Formula:

$$P = N k_b T / V + \sum_{i=1}^N (\mathbf{f}_i \cdot \mathbf{r}_i) / 3V \quad \text{http://lammps.sandia.gov/doc/compute_pressure.html}$$

Dimensionless form formula derivation:

Temperature:

$$T^* = \frac{T k_b}{\varepsilon} \Rightarrow T = \frac{T^* \varepsilon}{k_b}$$

Volume:

$$V^* = V \sigma^{-3} \Rightarrow V = V^* \sigma^3$$

Coordinates,

$$\mathbf{r}_i^* = \mathbf{r}_i / \sigma \Rightarrow \mathbf{r}_i = \mathbf{r}_i^* \sigma$$

force,

$$\mathbf{f}_i^* = \mathbf{f}_i \sigma / \varepsilon \Rightarrow \mathbf{f}_i = \mathbf{f}_i^* \varepsilon / \sigma$$

Pressure,

$$P^* = P \sigma^3 / \varepsilon \Rightarrow P = P^* \sigma^{-3} \varepsilon$$

Substitute into pressure computation formula, one obtains dimensionless form formula which is,

$$P^* = NT^* / V^* + \sum_{i=1}^N (\mathbf{f}_i^* \cdot \mathbf{r}_i^*) / 3V^*$$

See the excel file attached, please. The procedures to calculate temperature was given in excel file for time step 0 and 2 respectively.