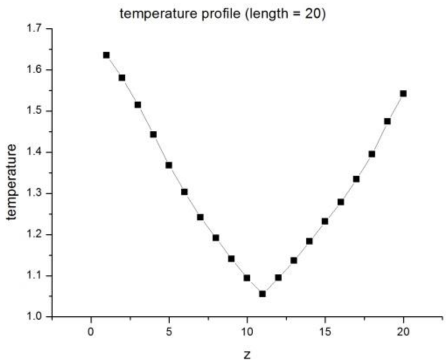
# thermostat

Length of a unit cell: l = $\sqrt[3]{4/0.6} = 1.882(sigma)$

Cross-sectional area of the tube: A = $l^2xy = 1.882^2 \times 10 \times 10 = 354.19(\text{sigma}^2)$

Length of the tube: L = lz = $1.882 \times 20 = 37.64$(sigma)

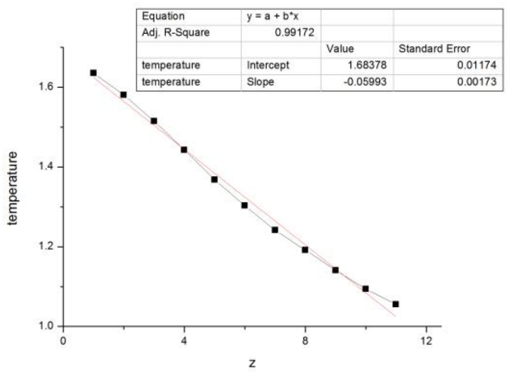
Temperature profile

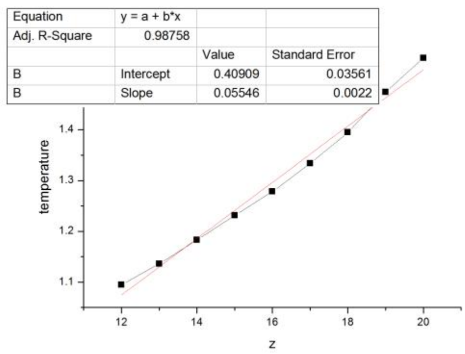



In order to deduce more reliable and steady temperature profile, sum over temperature value from 20000 to 31000 steps of each z point and use the average temperature.

The hot source locates on [0, 1]. The cold source locates on [10, 11]. When step number is large enough for the system to reach dynamic equilibrium (step = 31000, last set of data), according to the temperature profile, temperature approximately linearly declines from the hot source to the cold source.

Select data for z=[0, 11] and z=[11, 20], do linear fitting separately.

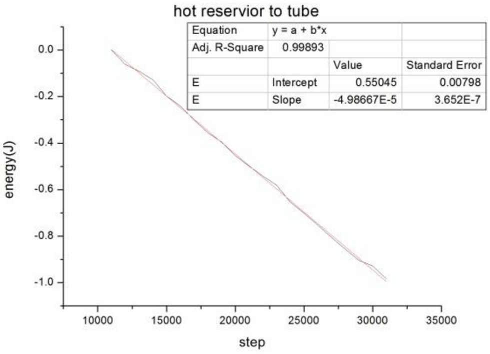


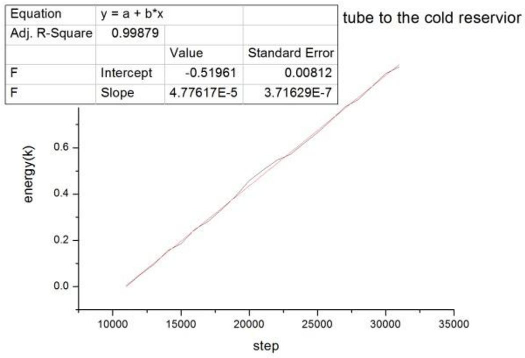




The average value of the absolute values of slop: $-\nabla T = (0.05993+0.05546)/ (2\times 1.882) = 0.0306$

Since the tube size is [10, 10, 20], its' cross-sectional area S = $10\times 10\times 1.882^2 = 354.19$ (sigma$^2$)

Energy exchange




Energy flow from the hot reservoir into the tube: $F_h = -4.98667 \times 10^{-2}/0.005$

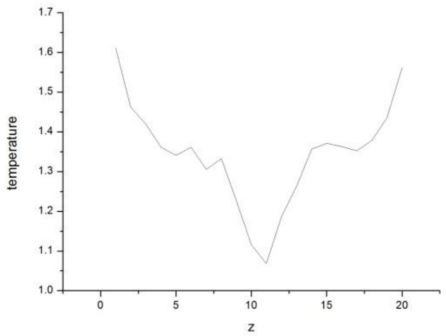
Energy flow from the tube into the cold reservoir: $F_c = 4.77817 \times 10^{-2}/0.005$

Average value of heat flow in the tube: $F = 4.88\times10^{-5}/0.005$

When L = 20, $k = \frac{F}{\Delta T} = 0.90$

Similarly, vary the tube length and obtain corresponding C:

| Length | 20 | 30 | 40 |
|---|---|---|---|
| k | 0.901 | 0.377 | 0.250 |



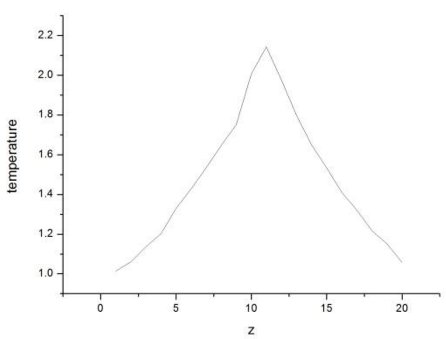

Heat capacity decreases as tube length increases.

As tube length increases, 31000 steps becomes insufficient for the system to reach thermal equilibrium state, hence run number should be increased to obtain credible thermal conductivity.

| t | 0.9 | 1.1 | 1.3 | 1.5 |
|---|---|---|---|---|
| C | 0.179 | 1.161 | 0.152 | 0.140 |

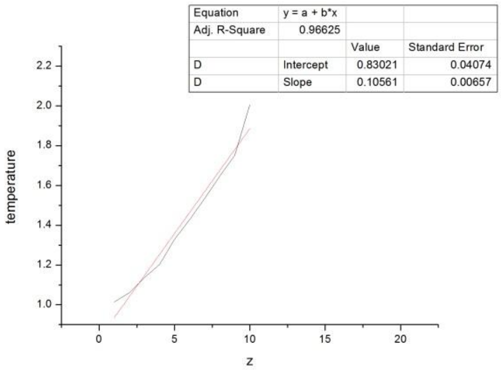
When average temperature increases, thermal conductivity decreases.

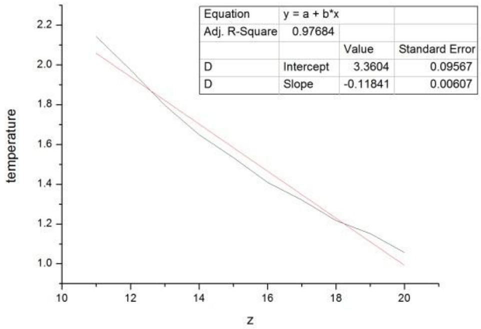
# Muller-plathe




Since in Muller-plathe method, energy is the largest for particles in the middle part of the tube and least on two ends, the temperature profile shows that approximately temperature linearly decreases from the center part of the tube to the end.

Select data for z=[0, 10], z=[11, 20]. Do linear fitting separately

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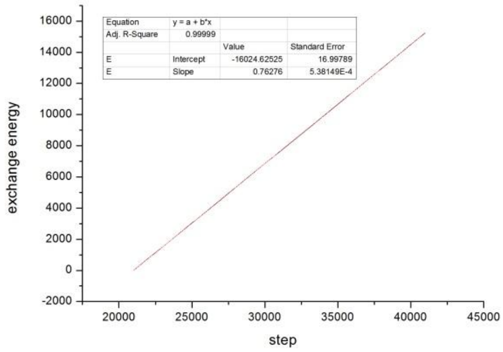
Length of the tube: L = lz = 1.882 × 20 = 37.64(sigma)

The average value of the absolute values of slop: ▽T = (0.10561+0.11841)/ (2×1.882) =0.0595

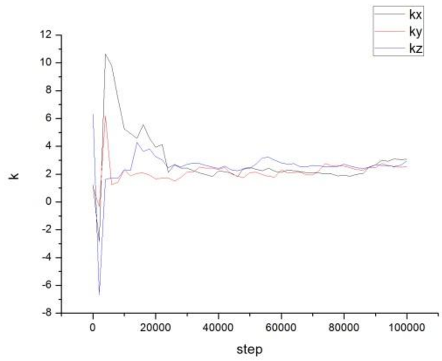



heat flow:

F = $\frac{enchange\ energy}{A \times timestep}$ = 0.76276/(354.19 × 0.005) = 0.4307

K = F/▽T = 7.24

# Green Kubo (z=10)




Time integration of <J(0)J(t)> first oscillate and reach to 2.62 as step increases.

Knowing $k = \frac{V}{k_B}\int_0^\infty < J_z(0)J_z(t) > dt$

According to result in log.lammps,
k= 2.85378774750157

Analyzing k deduced from three different method, the orders of magnitude are different but the values are close. The cause of this situation might be that lj is relevant unit.