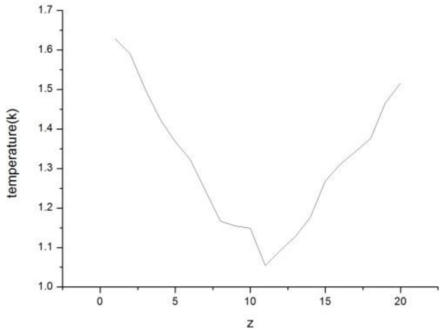
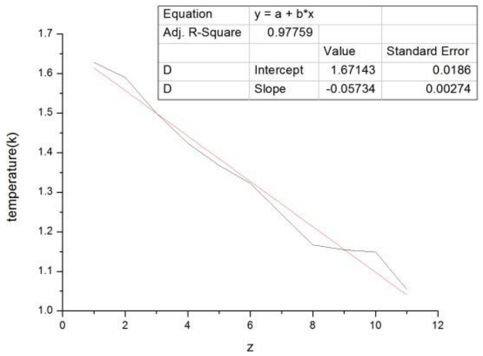
thermostat

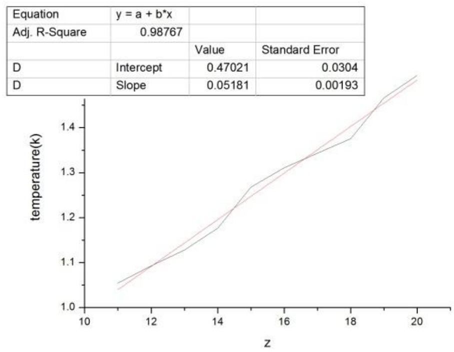
Temperature profile



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.

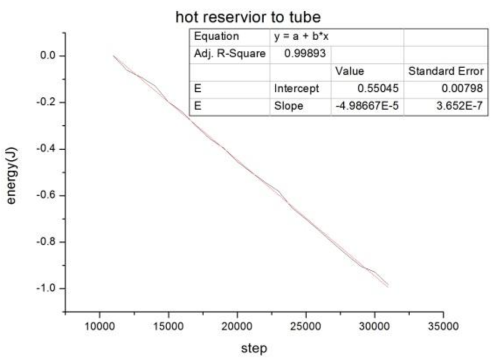


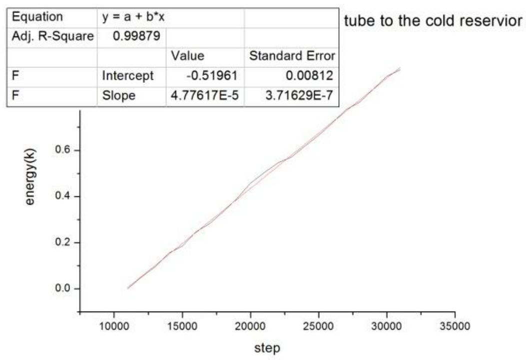


The average value of the absolute values of slop: $-\nabla T = (0.05734+0.05181)/ 2 = 0.0576$

Since the tube size is [10, 10, 20], its' cross-sectional area $S = 10 \times 10 = 100$ (A^2)

Energy exchange





Energy flow from the hot reservoir into the tube: $F_h = -4.98667 \times 10^{-5}/0.005$

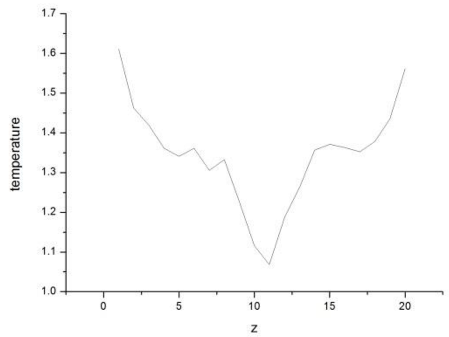
Energy flow from the tube into the cold reservoir: $F_c = 4.77817 \times 10^{-5}/0.005$

Average value of heat flow in the tube: $F = 4.88 \times 10^{-5}/0.005$

When L = 20 A, $C = \frac{F}{\nabla T} = 0.169$

Similarly, vary the tube length and obtain corresponding C:

Length	20	40	50	80
C	0.169	0.102	0.090	0.113

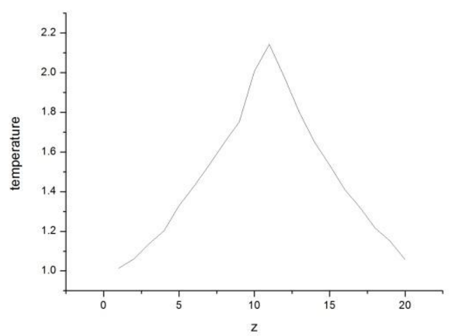


As tube length increases, 31000 steps becomes insufficient for the system to reach thermal equilibrium state, hence run number should be increased to obtain credible thermal conductivity.

t	0.9	1.1	1.3	1.5
C	0.179	1.161	0.152	0.140

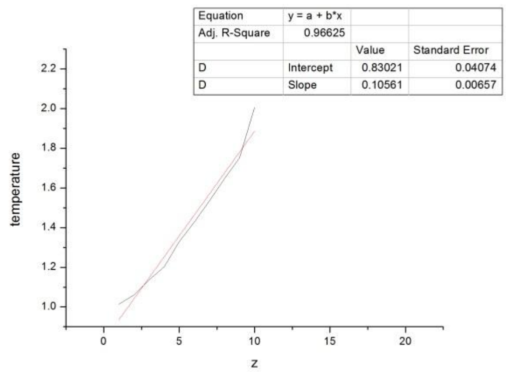
When average temperature increases, thermal conductivity decreases.

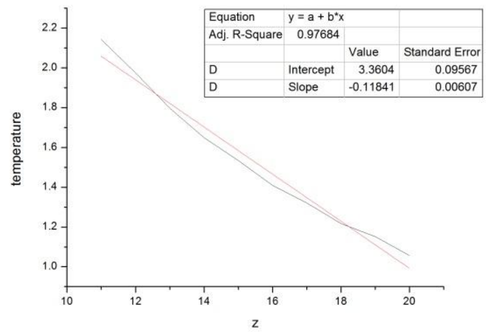
Muller-plathe



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.

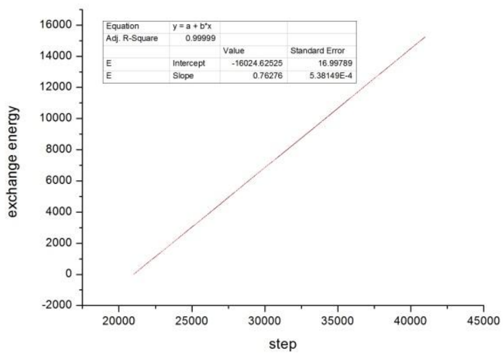
Select data for z=[0, 10], z=[11, 20]. Do linear fitting separately





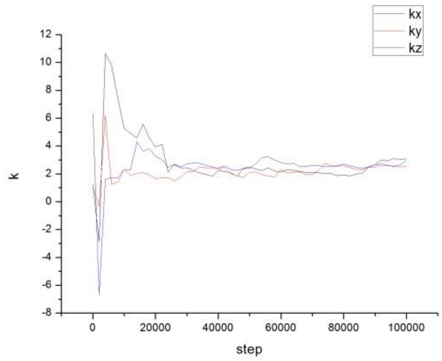
The average value of the absolute values of slop: $\bigtriangledown T = (0.10561+0.11841)/ 2 = 0.11201$

heat flow $F = 0.76276/0.005 = 152.552$



$C = F/\bigtriangledown T = 1362.0$

Green Kubo (z=10)



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

Knowing $k = \frac{V}{k_B}\int_0^\infty < J_z(0)J_z(t) > dt$ =1.90 × 10^{26}

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.