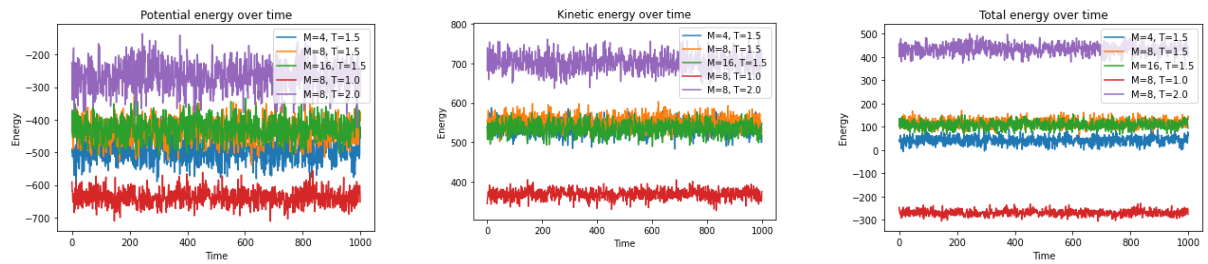# Ex8

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Trajectories

The .traj file can be found in the Gitlab repository

## Energies

Variances

	T = 1.5, M = 4	T = 1.5, M = 8	T = 1.5, M = 16
first phase of simulation (potential energy)	10877.437929306188	11309.229206166272	11110.082016710969
first phase of simulation (kinetic energy)	5330.514584564781	5241.076053496999	6053.052320754434
first phase of simulation (total energy)	293530.5669210919	266177.6533085348	255743.558046522
second phase (B) of simulation (potential energy)	1417.2441837954336	1295.2161490494505	1411.7964620242055
second phase (B) of simulation (kinetic energy)	380.3379340774787	352.2652636443329	386.7142418079769
second phase (B) of simulation (total energy)	270645.104661689	244747.1951296129	237349.39681651065
final phase of simulation (potential energy)	1165.960132197834	1106.7204362462437	1173.139464061328
final phase of simulation (kinetic energy)	291.41769530735485	276.6282882254088	293.21244055016706
final phase of simulation (total energy)	268917.81570507074	245559.43827410482	232757.33311927345

Mean-squared displacement

$$\frac{\sum_{i=1}^{N}(r_i - \bar{r})^2}{N}$$

Mean square displacement over time
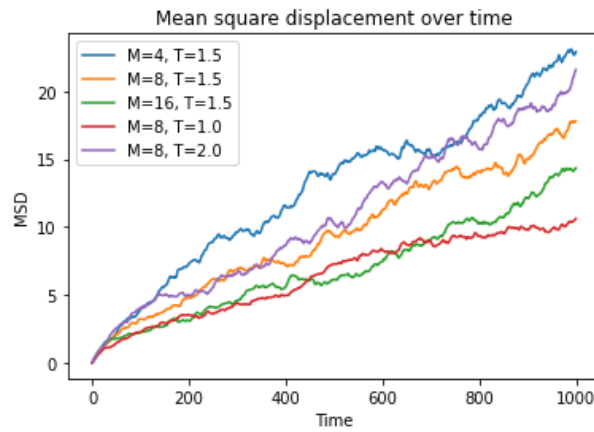
Diffusivity

	T = 1.5, M = 4	T = 1.5, M = 8	T = 1.5, M = 16	T = 1.0, M = 8	T = 2.0, M = 8
Diffusivity	0.03326437017593076	0.026586804672422342	0.020525346227717987	0.016656285234161485	0.03187806121926577

$$D = c \cdot T \cdot \exp\left(E_a / k_B T\right)$$
$$\Leftrightarrow c = \frac{D \cdot \exp\left(-E_a / k_B T\right)}{T}$$
$$\rightarrow c_1 = c\left(T_1, D_1\right)$$
$$c_2 = c\left(T_2, D_2\right)$$
$$c_3 = c\left(T_3, D_3\right)$$
$$c_1 \overset{!}{=} c_2 \overset{!}{=} c_3$$
$$c_1 = c_2 \rightarrow E_{a,1} = -0.5594605462$$
$$c_2 = c_3 \rightarrow E_{a,2} = 1.911223136$$
$$c_1 = c_3 \rightarrow E_{a,3} = 0.2641006811$$
$$\langle E_a \rangle = 0.5386210903$$
$$c1 = 0.01391889505$$
$$c2 = 0.01572507141$$
$$c3 = 0.01457052533$$

With that you can say that

$c_1 \approx c_2 \approx c_3$

And so D is proportional to the given expression.