FINDING A MODEL FOR SIMULATING THERMOPHORESIS

COMPUTATIONAL PHYSICS FINAL PROJECT

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THE MAIN QUESTION

What will happen if we put a macro particle in a pool of micro particles which are located between two walls with different temperatures?

THE COORDINATES, SPACE AND BOUNDARY CONDITION

- 2D box
- Periodic Condition
- Some regions along the horizontal axis

THE MICRO PARTICLES

- They do not have radius (The probability of collision between them is zero).
- Number of micro particles

A MODEL FOR INTERACTION BETWEEN MICRO PARTICLES IN ORDER TO GENERATE TEMPERATURE GRADIENT

- They do not see each other (There is no interaction between them).

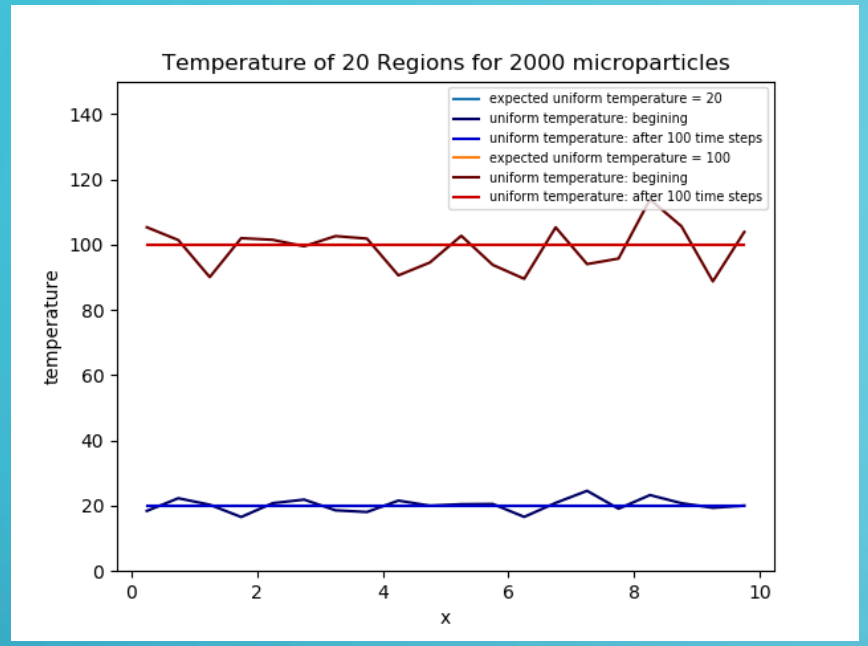
$$T = {E_k}/{N \times k}$$

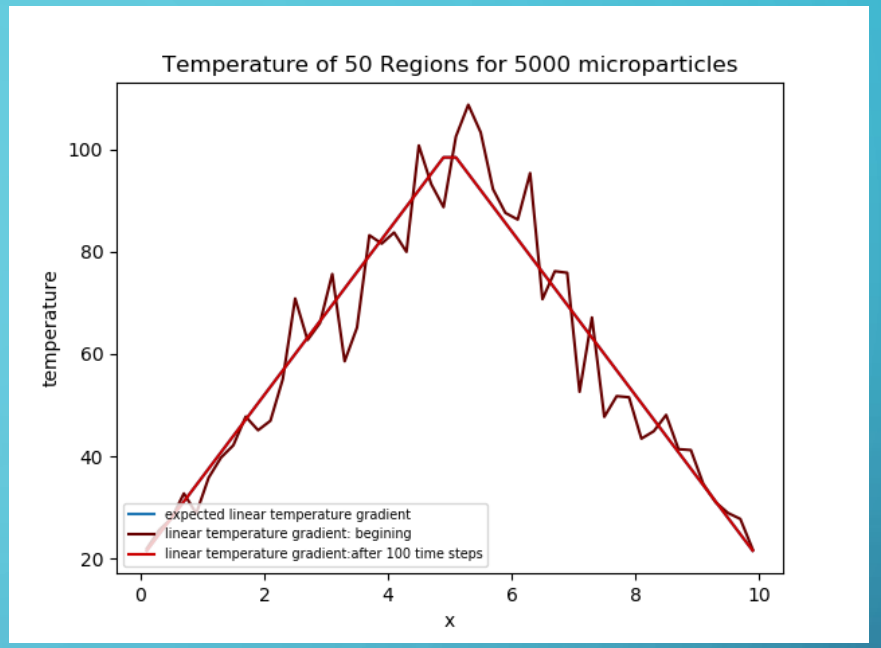
- Thermostat

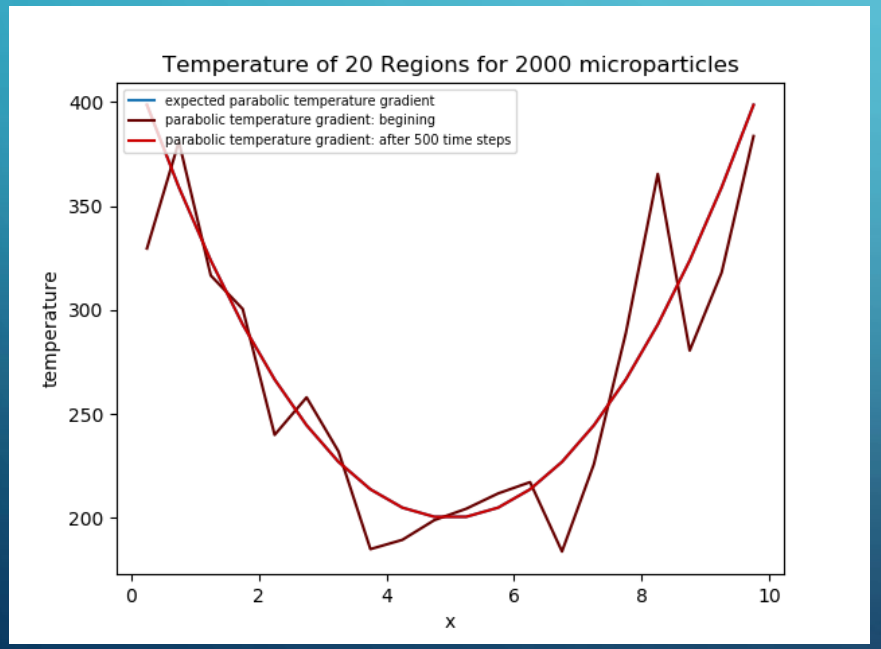
$$\text{Correction Coefficient} = \sqrt{(N \times k \times T)/E_k}$$

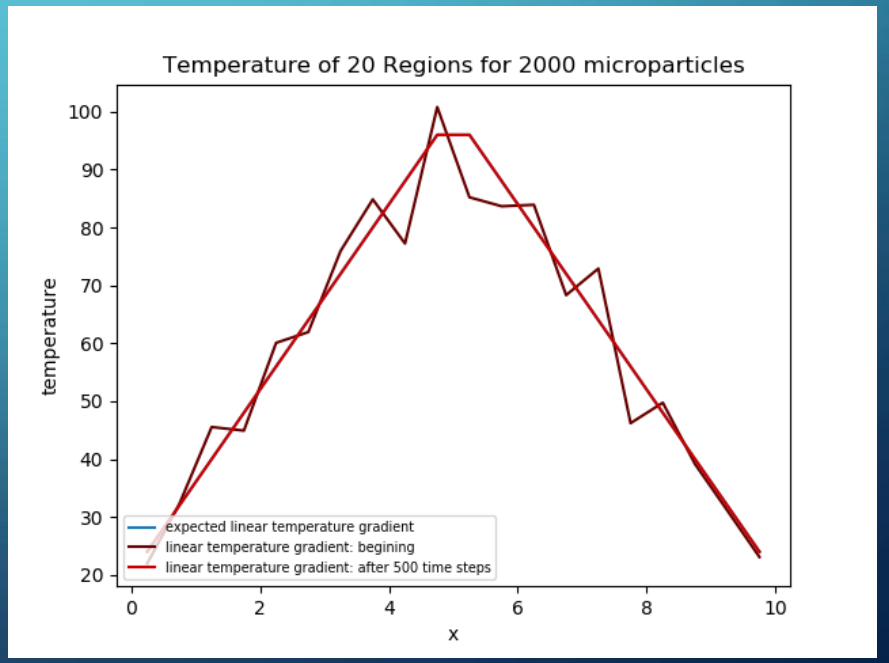
- Uniform random distribution for initial locations
- Boltzmann distribution for initial velocities

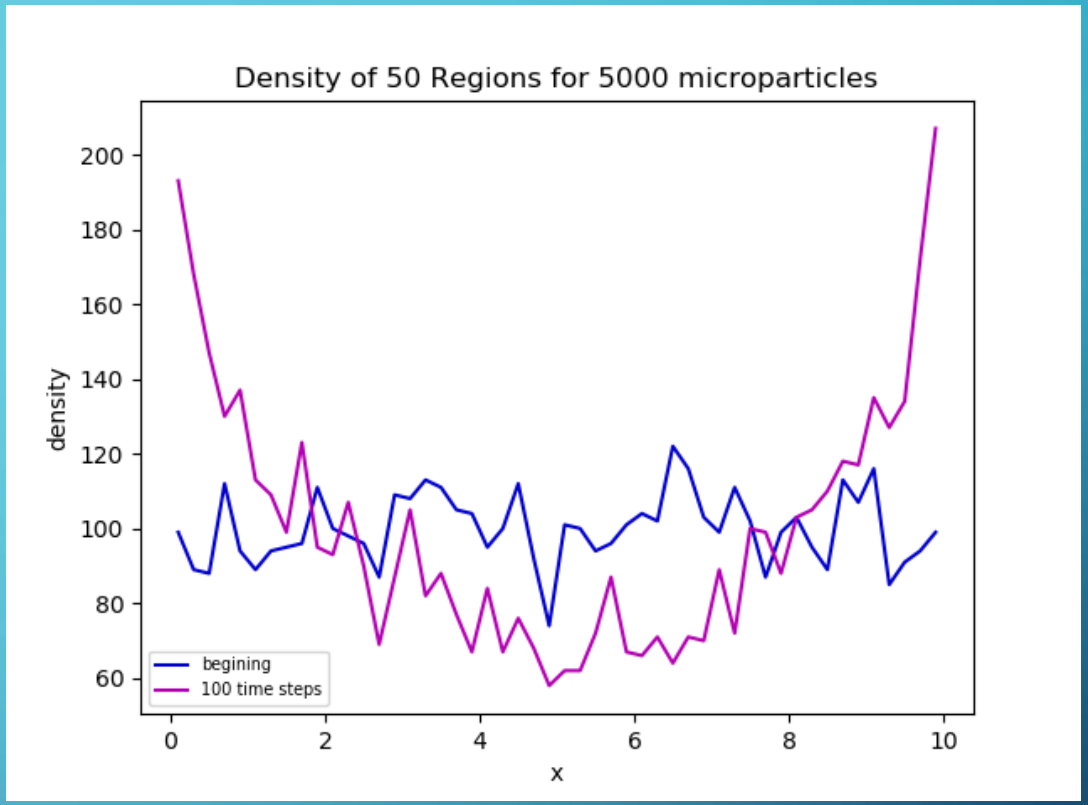
$$e^{-E_k/kT}$$

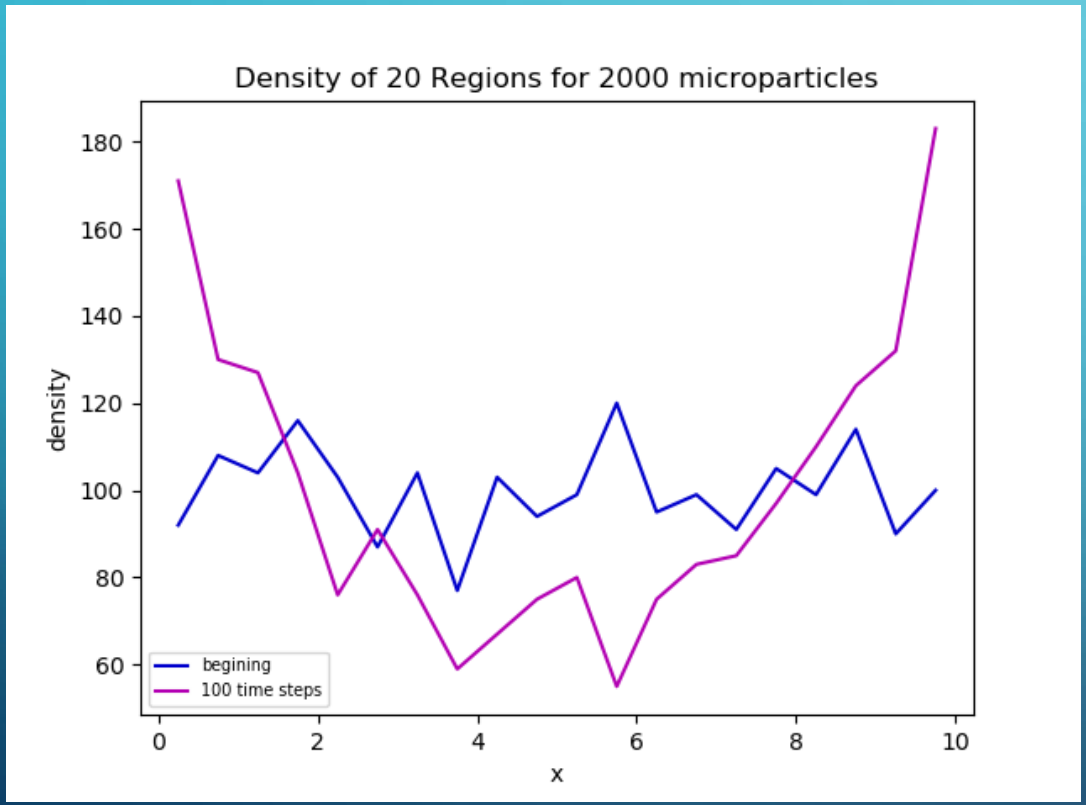

Temperature of 20 Regions for 2000 microparticles
expected uniform temperature = 20
uniform temperature: begining
uniform temperature: after 100 time steps
expected uniform temperature = 100
uniform temperature: begining
uniform temperature: after 100 time steps
temperature
x


Temperature of 50 Regions for 5000 microparticles
expected linear temperature gradient
linear temperature gradient: begining
linear temperature gradient:after 100 time steps
temperature
x

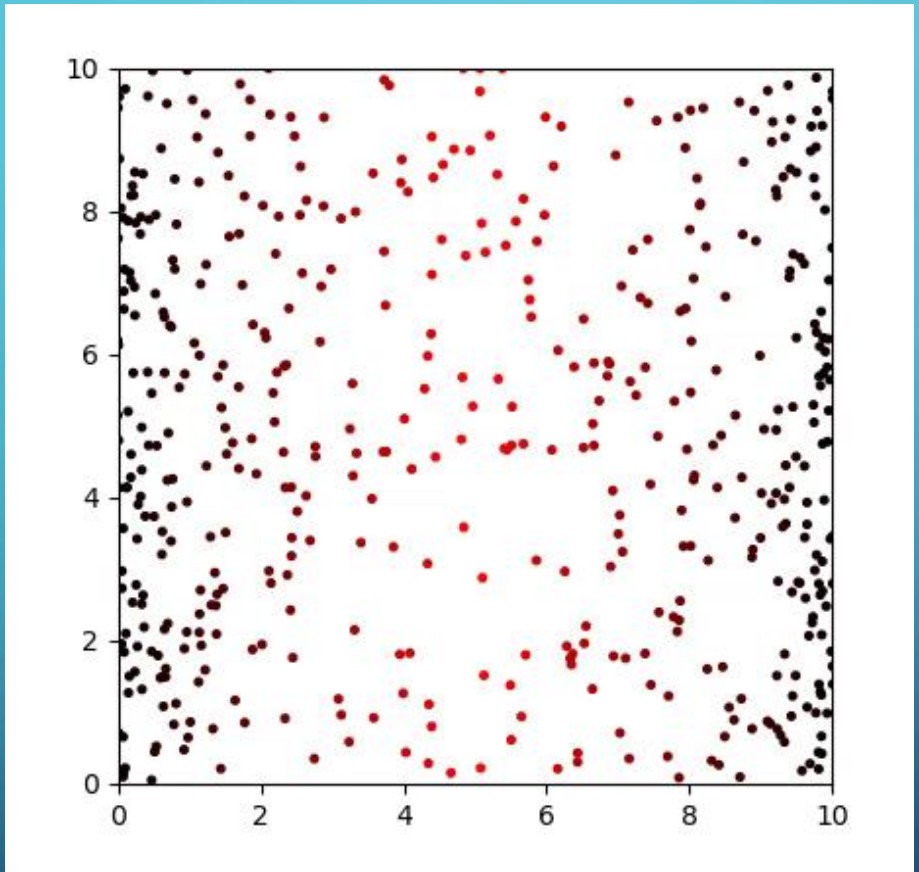

Temperature of 20 Regions for 2000 microparticles
expected parabolic temperature gradient
parabolic temperature gradient: begining
parabolic temperature gradient: after 500 time steps
temperature
x


Temperature of 20 Regions for 2000 microparticles
expected linear temperature gradient
linear temperature gradient: begining
linear temperature gradient: after 500 time steps
temperature
x


Density of 50 Regions for 5000 microparticles
density
x
begining
100 time steps
200
180
160
140
120
100
80
60
0
2
4
6
8
10

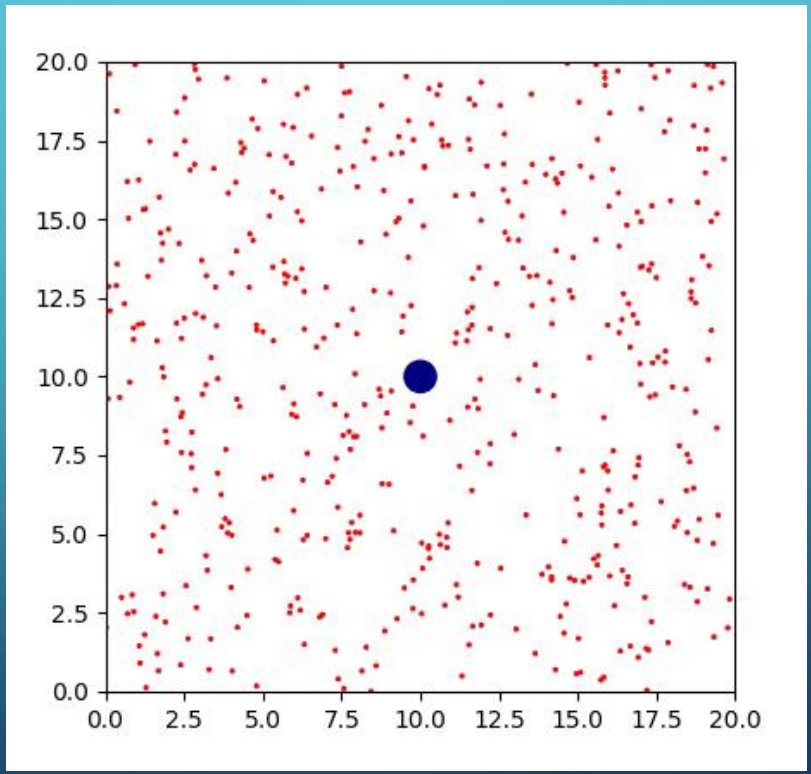

Density of 20 Regions for 2000 microparticles
density
x
begining
100 time steps
180
160
140
120
100
80
60
0
2
4
6
8
10

500 MICRO PARTICLES IN 50 REGIONS

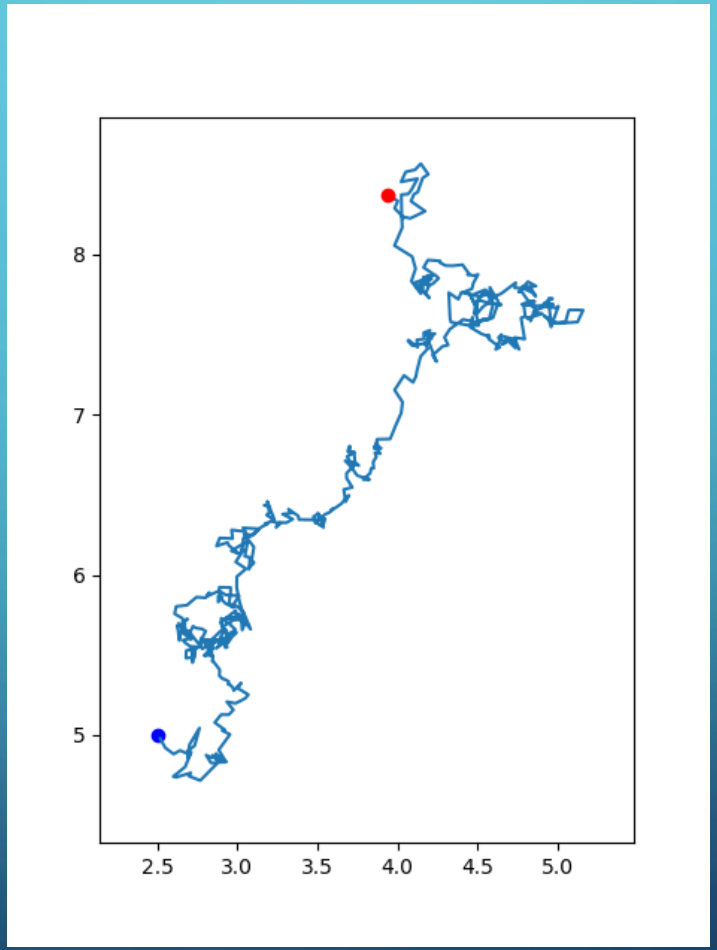


A MODEL FOR INTERACTION BETWEEN MICRO PARTICLES AND MACRO PARTICLE

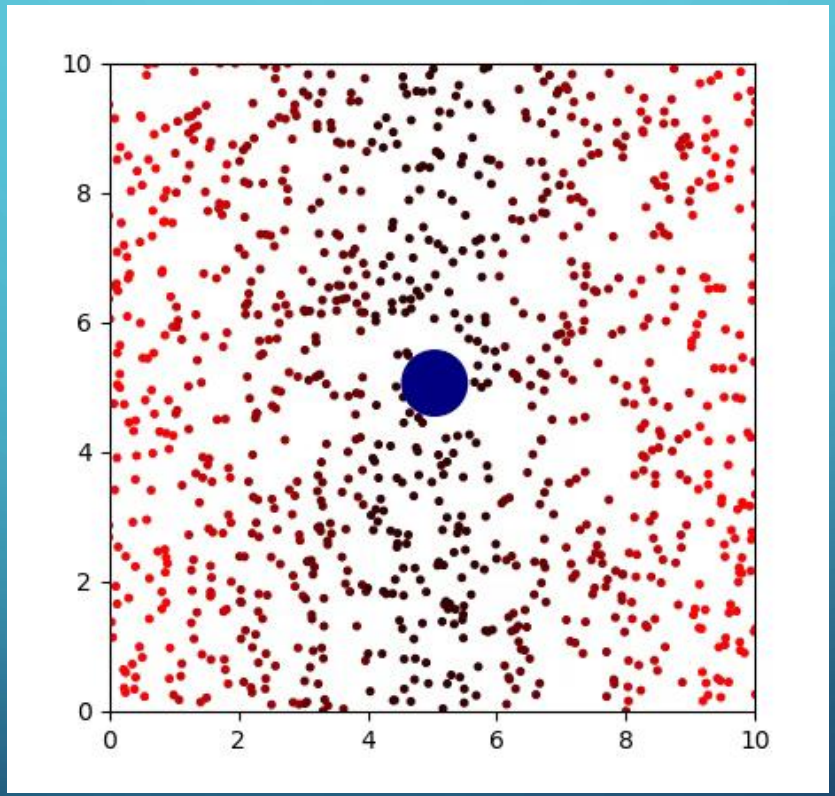
- Energy and Momentum is conserved (Elastic Collision).



MOTION OF THE MACRO PARTICLE UNDER UNIFORM TEMPERATURE



MOTION OF THE MACRO PARTICLE UNDER PARABOLIC TEMPERATURE GRADIENT



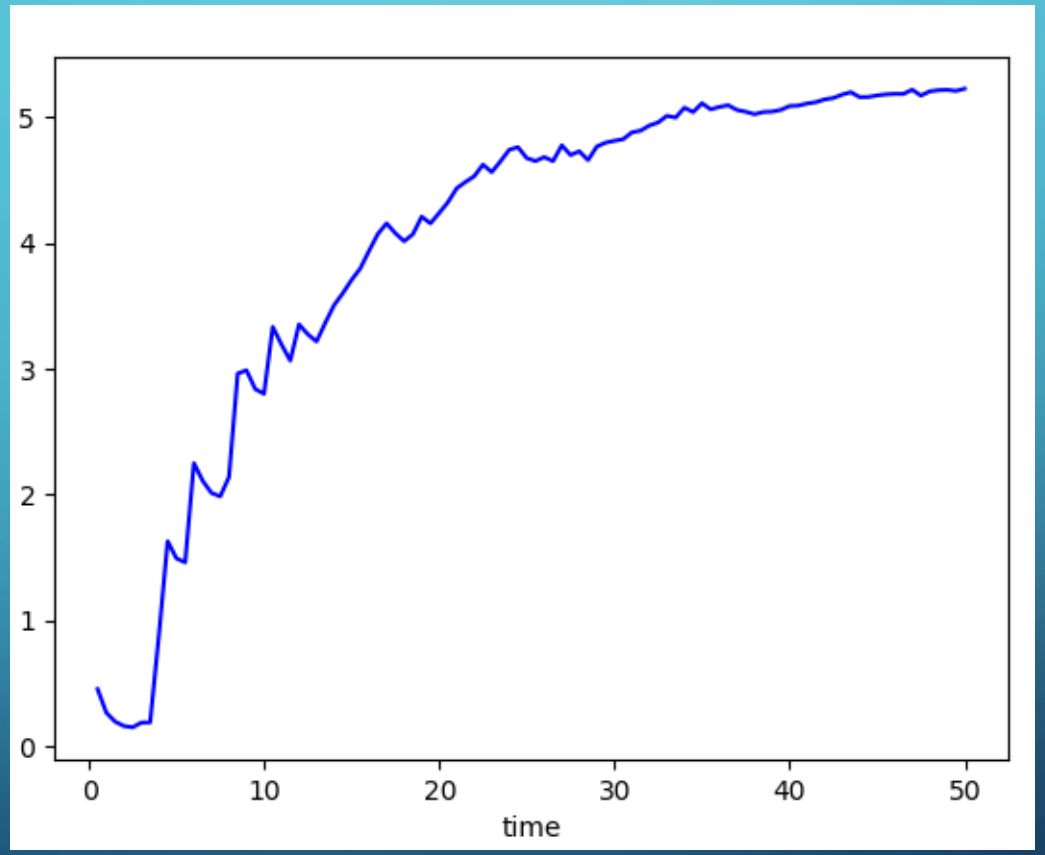
HOW TO VERIFY THE MODEL

- Energy conservation? No
- Momentum conservation? No
- Brownian motion

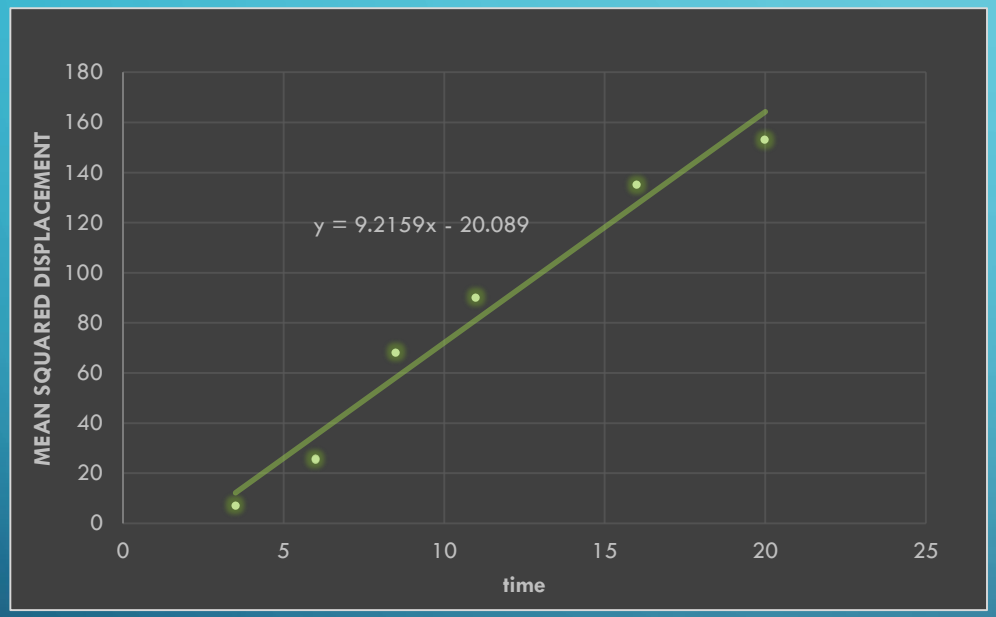
$$\text{MEAN SQUARED DISPLACEMENT} = 2D \times time$$

$$D = {}^{kT}/_{6\pi\eta r}$$

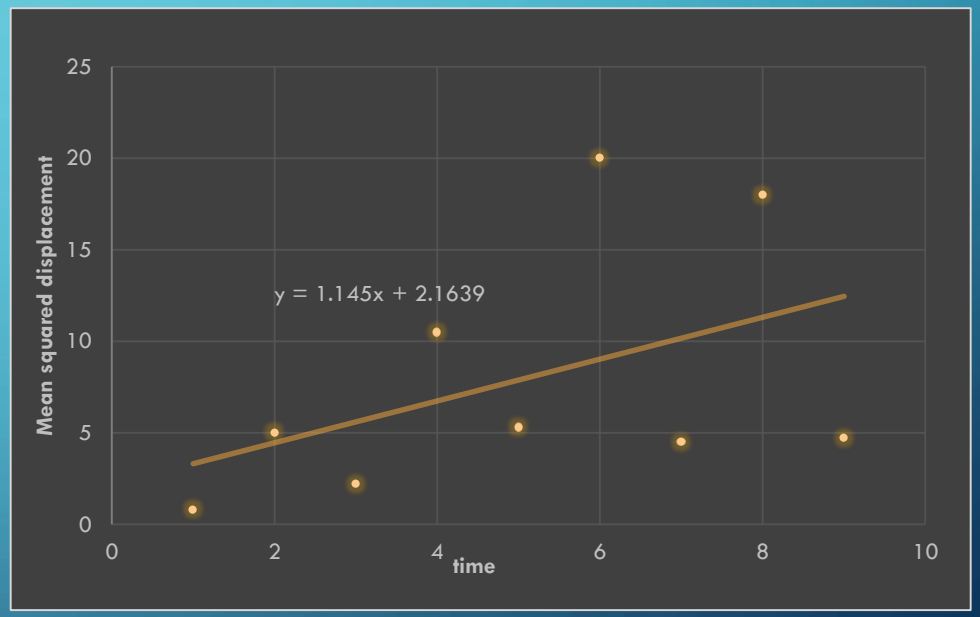
BROWNIAN MOTION?!



BROWNIAN MOTION?!



r = 0.5



r = 5