# Comp Phys Report 9:Differential Equations

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June 22, 2023

## 1 class MolecularDynamic

the class to simulate Molecular Dynamic model with Monte Carlo algorithm. Cause we are using NVT ansamble in this simulation to initialize the object of this class we have to set N (the number of particles), length ( the length of the box ) and T as the temperture of the system also we are using lenard jones potential between particles with a cut off distance (

$$r_c = 2.5 * \sigma$$

) so we have to define

$$\sigma$$

and

$$\epsilon$$

for the potential in monte carlo algorithm we have a jumping param that i represented it with delta.

in order to set all particles in the left side of the box i find a length param a that represents the distance between particles at initial condition and with that param i created some positions by splitting the left side into new squares and then took N of them

then i got the

$$U_{net}$$

of system which i'll gonna explain later.

### 1.1 methods

#### 1.1.1 run

this is the main method of the simulation.to run the simulation we have to get the T for ansamble and delta for Monte Carlo algorithem. then in monte carlo we choose one particle,get one shift in space and times with delta and get a third random value,all of them should be random

then i initialize trajectories to store data in them

then in the main loop i have bigSteps and smallSteps

each bigStep includes a lot of smallSteps and after each bigStep i store data in trajectories.

#### 1.1.2 step

this method represents each update of the system. first i copy the positions and add the shift on

$$th$$

particle then i check if the particle is not out of bounds

after that i calculate the distance between particles which is a

$$N * N$$

matrix of complex values. i use complex values which real part is on first axis and the imaginary part is on second one then find the magnitude of the distances between particles and filter the ones which are farther than

$$r_c$$

then with new distances we can find the new potential of the system and accept the changes of positions and potential if monto carlo condition is true

if

$$dU = U_{new} - U < 0$$

or

$$randomValue < exp(-dU/k_B * T)$$

then the condition is true.(

$$k_B = 1$$

)

#### 1.1.3 getLeftSidedNum

this is the method to check the first axis of the position of the particles and count if its less than

$$L/2$$

#### 1.1.4 animate

the method to animate the input trajectory. i create on image after the interval and save it,then transform all images into one video

#### 1.1.5 getDistanceMatrix

the method to find the distances between each particle. i tile the positions up and and subtract the positions with one shift

then in order to find the min distance of all images of particles in infinite space i used reminder

$$(distance + L/2)\%L - L/2$$

gives the min of distances

#### 1.1.6 getU

lenard jones potential is

$$U(r) = 4 * \epsilon((\sigma/r)^1 2 - (\sigma/r)^6)$$

to get

$$U_{net}$$

i got U(rMag), deleted the values of nan (cause

$$r_{ii} = 0$$

) and filter the far ones and divide it by 2 cause i counted each couple two times

#### 1.1.7 getRebounded

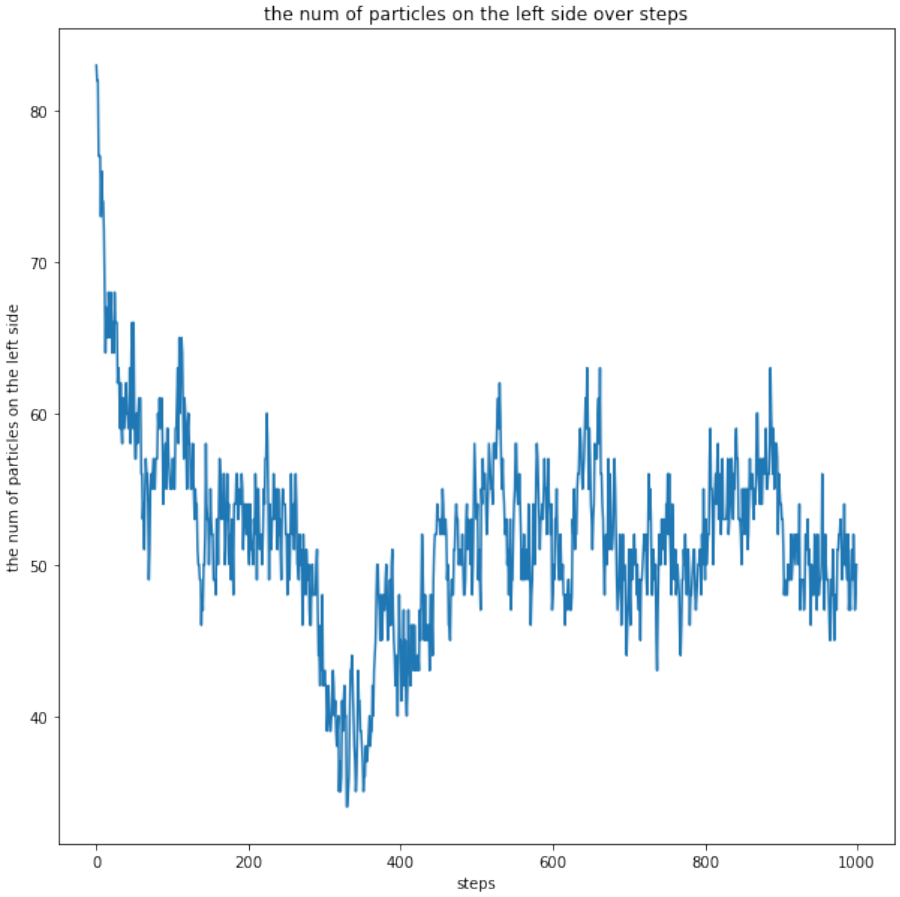
the method to return the reminder of the input array on L in order to rebound the positions

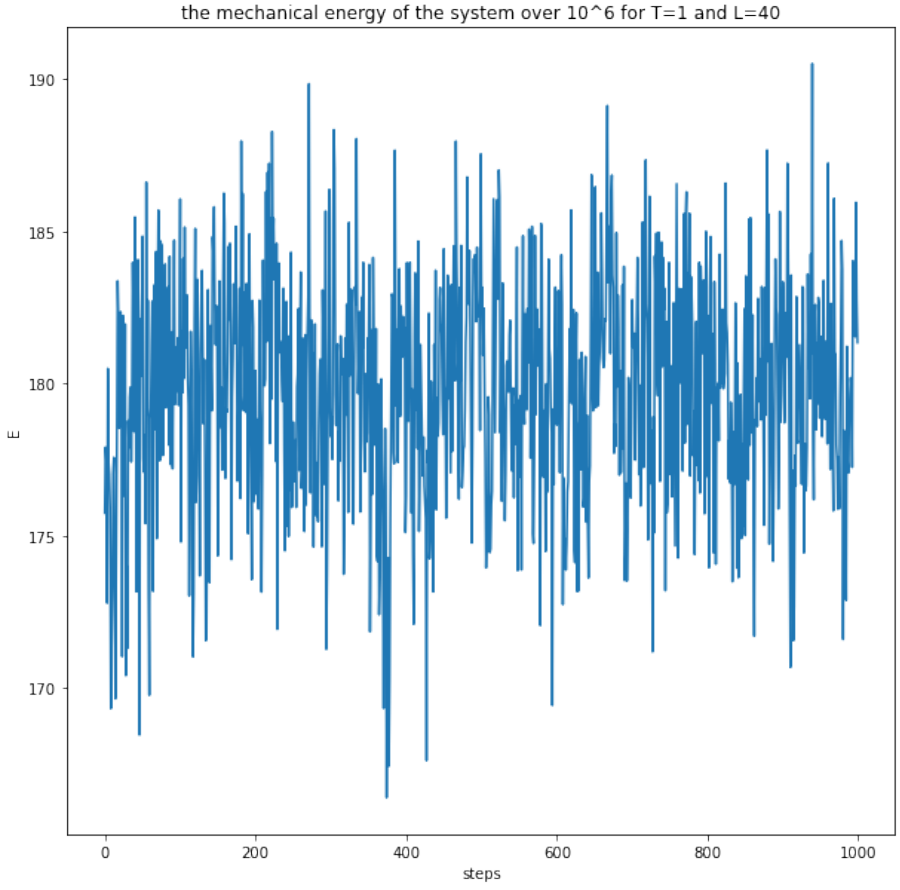
### 1.2 Results

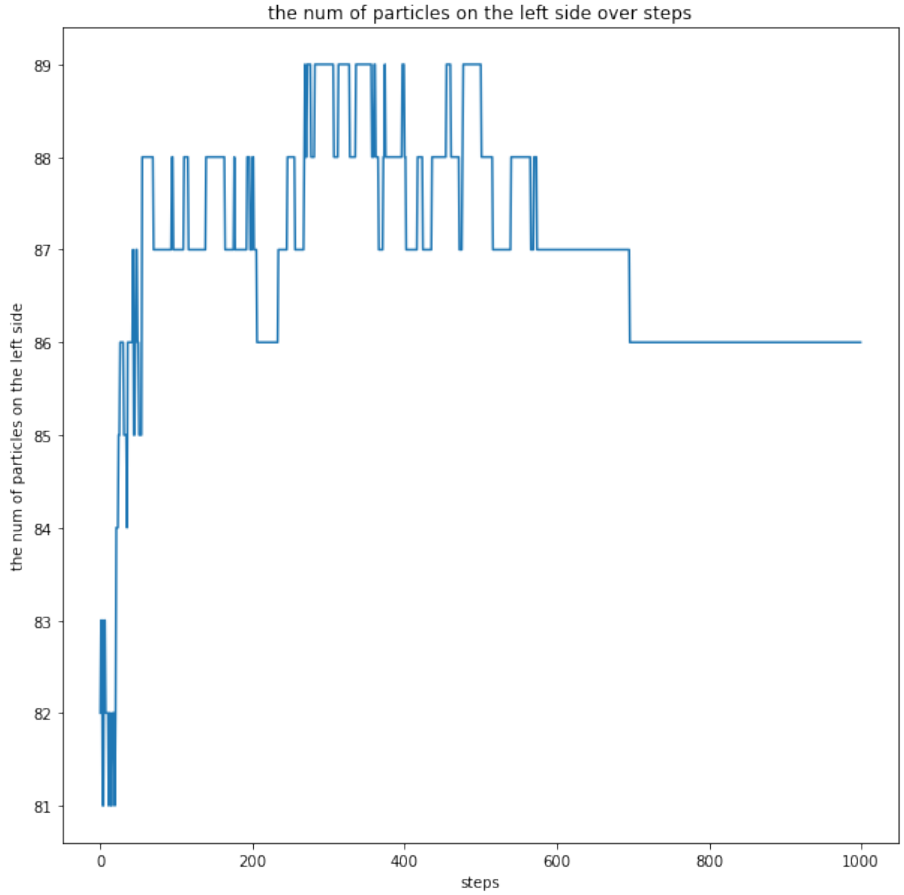
i simulated with params bellow and plotted the leftSidedNumber and E trajectory which is U trajectory + 2NT as its shown in animation there are many sold clusters when T is low.

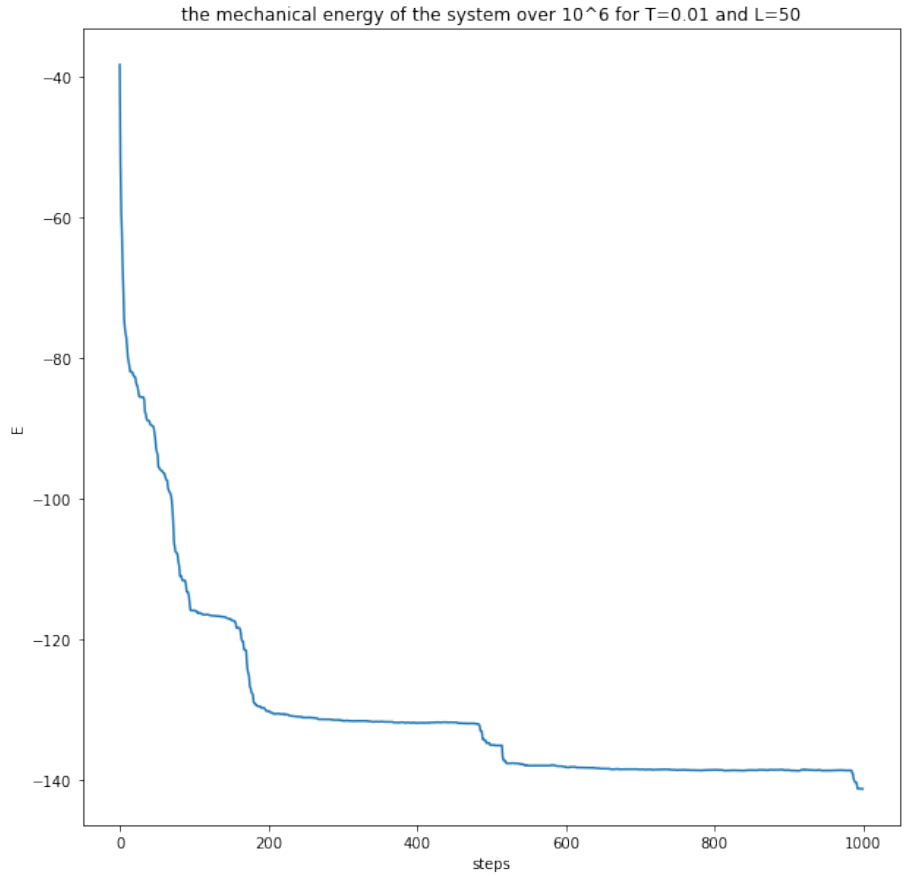
$$N = 100\sigma = 1\epsilon = 1L = 40bigStep = 1000smallStep = 1000T = 1delta = 1$$

$$N = 100\sigma = 1\epsilon = 1L = 50bigStep = 1000smallStep = 1000T = 0.01delta = 1$$


the num of particles on the left side over steps
the num of particles on the left side
steps
80
70
60
50
40
0
200
400
600
800
1000


the mechanical energy of the system over 10^6 for T=1 and L=40
E
steps
190
185
180
175
170
0
200
400
600
800
1000


the num of particles on the left side over steps
the num of particles on the left side
steps
89
88
87
86
85
84
83
82
81
0
200
400
600
800
1000


the mechanical energy of the system over 10^6 for T=0.01 and L=50
E
steps
−40
−60
−80
−100
−120
−140
0
200
400
600
800
1000