Computational Physics Homework Report

Fateme RamezanZade-99100693 Problem Set 11

1. Functions Description

Init(n,L,v_max):

This function is responsible for setting up the initial conditions. It puts all of the n number of particles in a lattice in the left side of the box, then assigns a velocity in range (-v_max,v_max) to each of them both in x and y axis. Then returns the arrays of x and y positions and velocities.

Accel(x_arr,y_arr,L):

This function calculates the total force applied to a particle in each direction. It gets the positions of particles and the size of the box in advance, then for each particle in each direction, repeats this process to store the value of f_ij in a matrix: finds the distance of each particle from it (if the distance is larger than the cutoff distance, uses its nearest mirror image), then calculates the force which is excerted from this particle to it and sorts it in an array. It fills the other triangle half of the matrix just by multiplying the values already calculated with a minus. Lastly, returns the sum of each row as the total force exsserted to i'th particle and also the forces matrix.

Verle(h,N,x_0,y_0,vx_0,vy_0,L):

This function uses verle algorithm and calculates the position and velocity after N steps with step size h.

potential(x_arr,y_arr,L):

This function calculates the distance between each pair of particles, the same way in the accel function, then calculates their potential. Lastly, returns an array which consists of the potentials of each particle.Kinetic(vx_arr,vy_arr):This function simply uses the values of velocities and returns the kinetic energy of each particle stored in an array.

Virial(x_arr,y_arr,L):

This function is responsible for calculating the value of this term which is needed to find pressure with virial expansion:

$$\sum_{i}^{n}\sum_{j>i}^{n} r_{ij}.f_{ij}$$

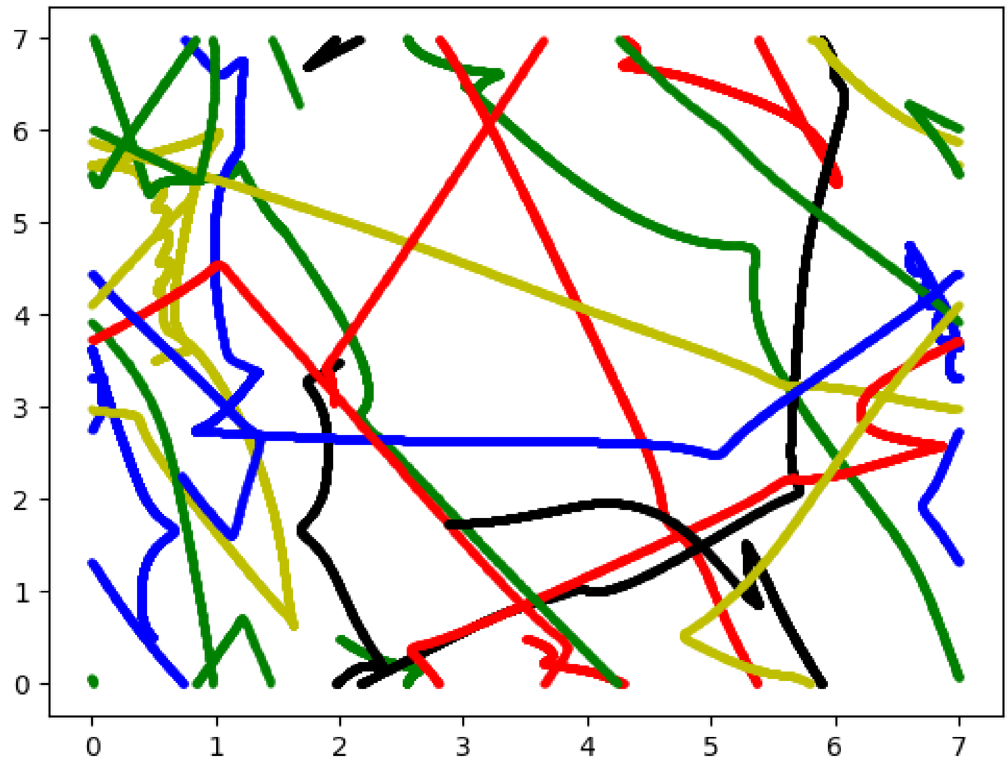
2. Results:

In all of the following parts, the dynamics of 100 particles in a box with size 30*30 is simulated, and the range of velocities in each direction is (-1,1) except it is mentioned otherwise. Also, in order to find kinetic energy, I subtracted the center of mass velocity from each velocity and did it in the rest frame of the box.

2.1. Trajectories

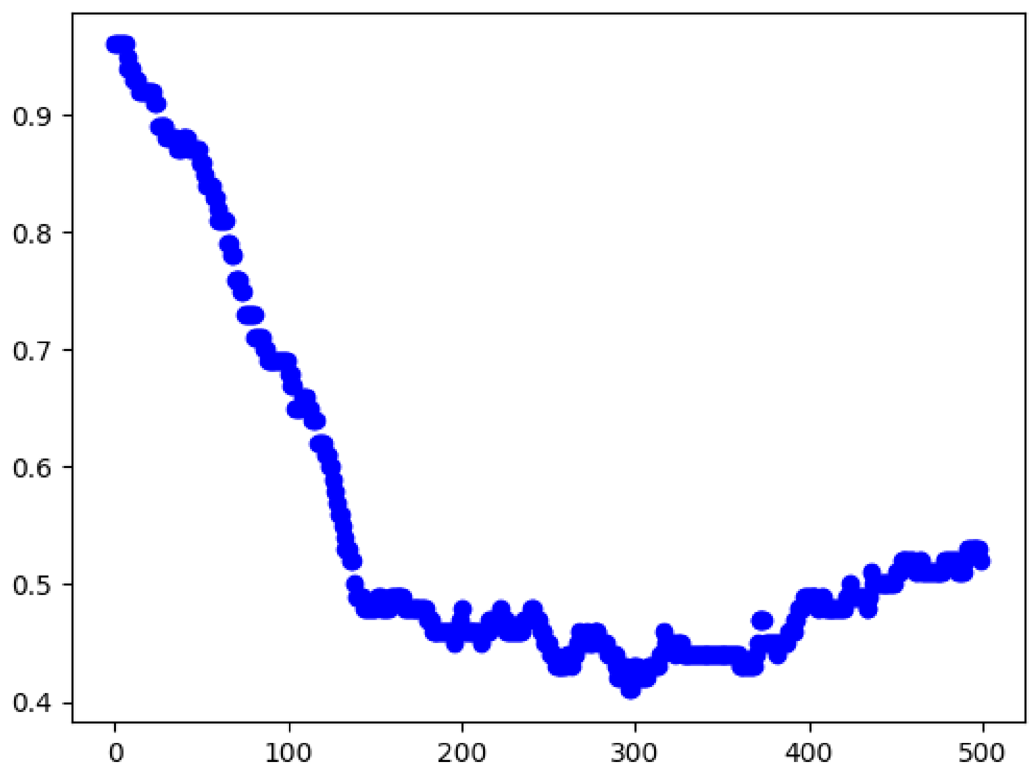
After initializing the system, the positions of particles are stored after each 5 steps. The step size is 0.001 and the total number of steps is 5000 times.

For this part, I just plotted 5 particles in a 7*7 box so that trajectories are recognizable.



From now on, after initializing the system, the positions of particles are stored after each 10 steps. The step size is 0.005 and the total number of steps is 5000 times.

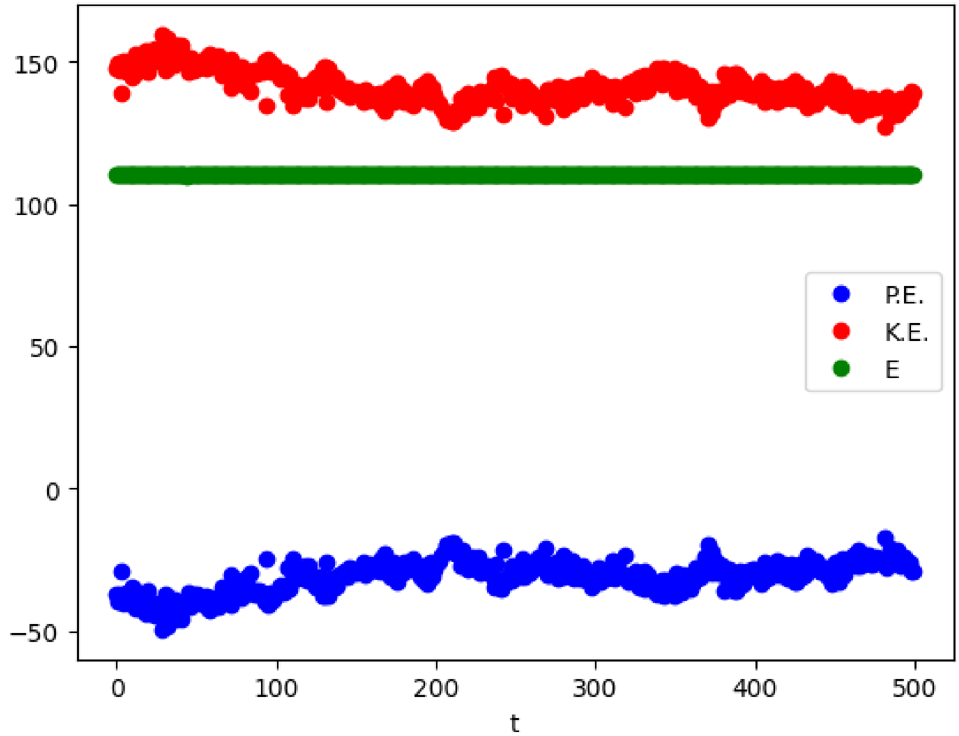
2.2. Number of Particles in the Right Half



We can see that after the relaxation time, the ratio of the number of particles in each half to the total number would be equal.

2.3. Energies

We can notice that the total energy remains constant.



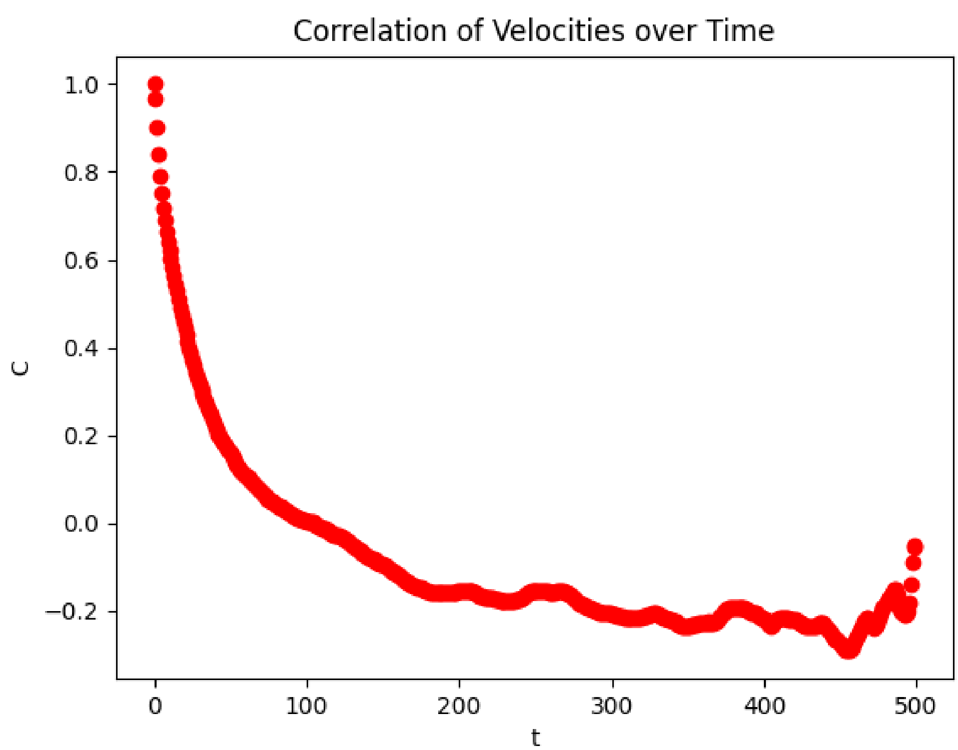
2.4. Velocity Correlation

We know that the autocorrelation function of speeds, has this formula:

$$C(t) \sim e^{-\frac{t}{t_r}}$$

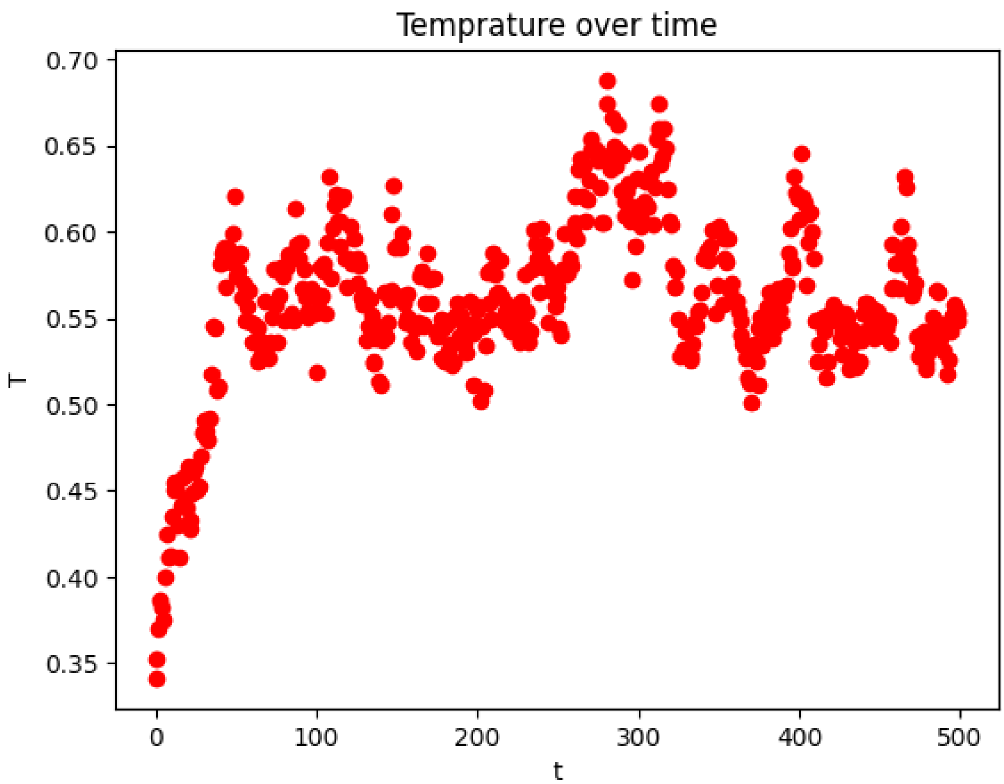
Where t_r is the relaxation time.

$\tau = 24.6 \times 0.005 \times 10 = 1.23$(reduced unit of time)

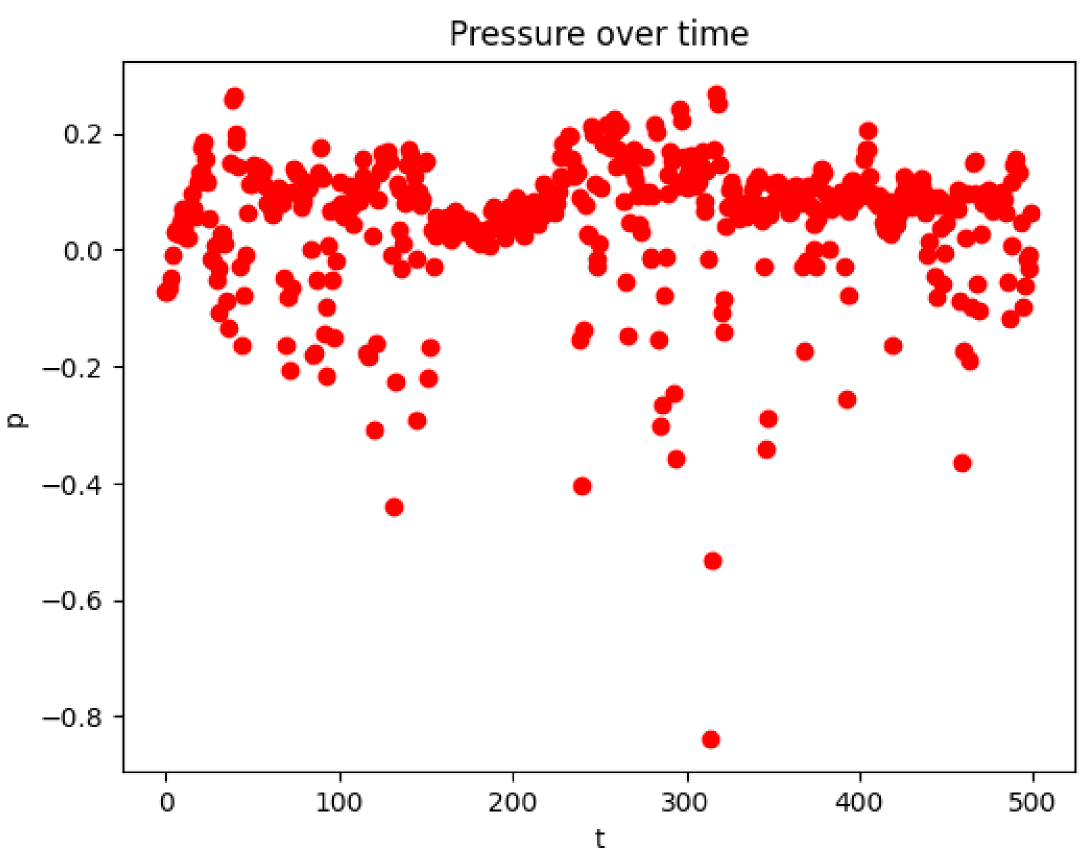


2.5. Temperature and Pressure

We can calculate the temperature after the relaxation time, which is about 0.56 in our reduced units.



Also, the pressure would be about 0.069. It is worth mentioning that in order to achieve the values, the outliers are excluded from the last 200 elements of the arrays using the function (reject_outliers) which I found online; and the mean of it is reported.



2.6. Van der Walls Coefficients

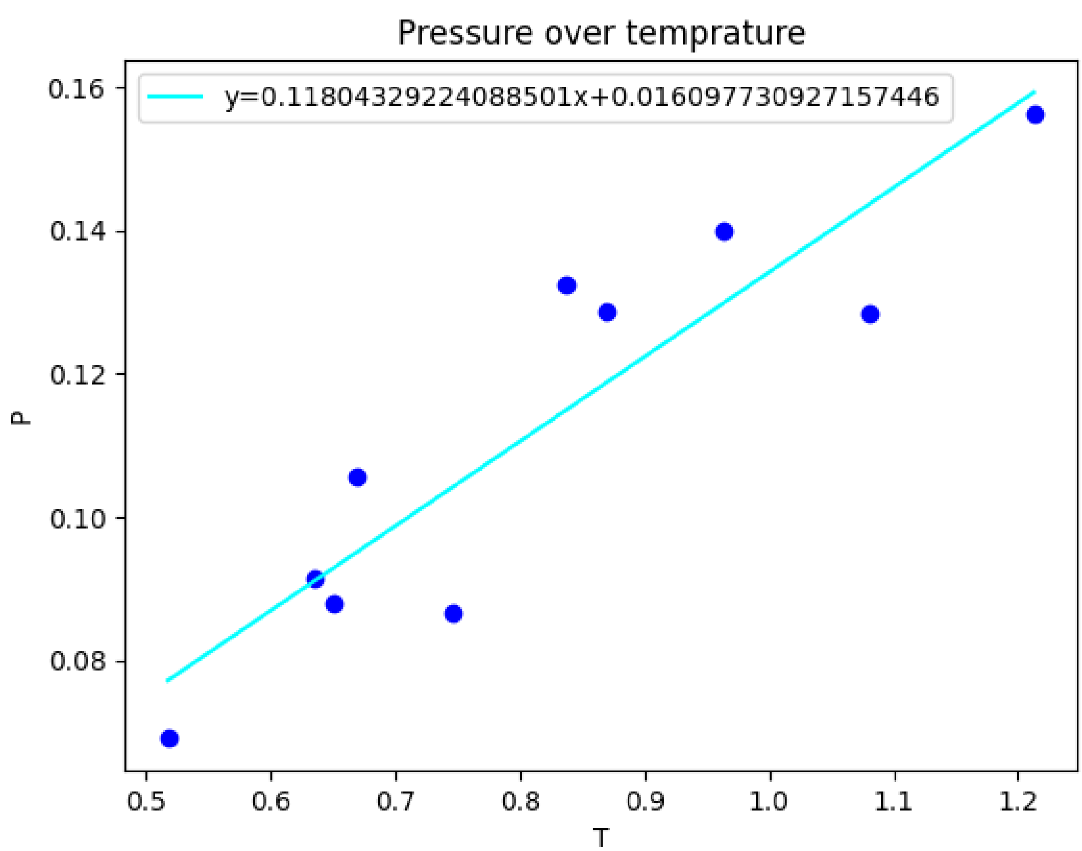
For ten different maximum initial velocities, in range (1,2), I calculated the temperature and pressure the same way as the previous part. Then I plotted the graph of temperature over pressure to find van der walls coefficients using this relation:

$$P = \frac{T}{\frac{L^2}{N} - b} - \frac{N^2}{L^4}a$$

Thus we would have:

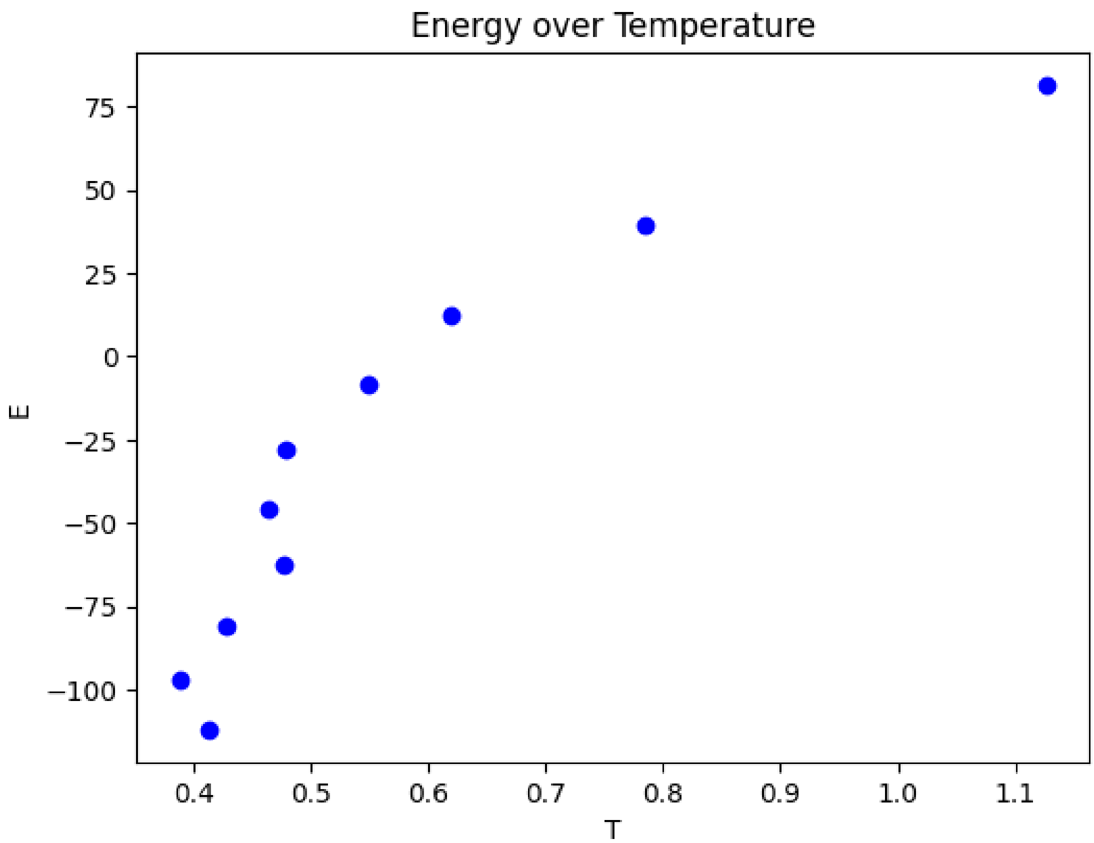
$$\frac{10^4}{30^4}a = 0.016 \Rightarrow a = 1.29$$
$$\frac{1}{\frac{30^2}{100} - b} = 0.118 \Rightarrow b = 0.52$$

In reduced units.



2.7. Phase Transition

For this part, after obtaining the temperature and Energy for one initial condition, I scaled the final velocities with 0.8 and set them as the new initial conditions, and tepeated that for 10 times. We can see that after a certain amount of repeats, the energy drops drastically. This can tell us that a phase transition from the gas phase has occurred.



Energy over Temperature
75
50
25
0
−25
−50
−75
−100
E
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
T