22.53 Problem Set IV solution

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October 16, 2000

1 Problem 9

Generally speaking, MC simulation is energy-based while MD simulation is force-based. MC calculation should be faster than MD calculation. Of course, if we want to compare some quantity in MC calculation with the result of MD calculation, it will depend on the accuracy we want. Also, there is a problem that which quantity can be regarded as the correct one. Therefore, we don't compare the results but compare the running time at given running steps. The results are as followings:

Testing Environment: on the machine of ATHENA.DIALUP.MIT.EDU
Testing Conditions: 256 particles,
2000 time-steps for MD and 2000 move-steps for MC.
MD program running time = 130 seconds;
MC program running time = 80 seconds.
It can be seen that MC program does have a better computational speed. This agrees with our above discussion. The force calculation is much time-consuming than the energy calculation. In our MC code, there is still one place where we can improve our computational speed. In the energy calculation to judge the validity of trial move, we can calculate the potential energy change only. I have calculated the total potential energy any way. But actually, we can only calculate the property of interest. That will save a lot of time.

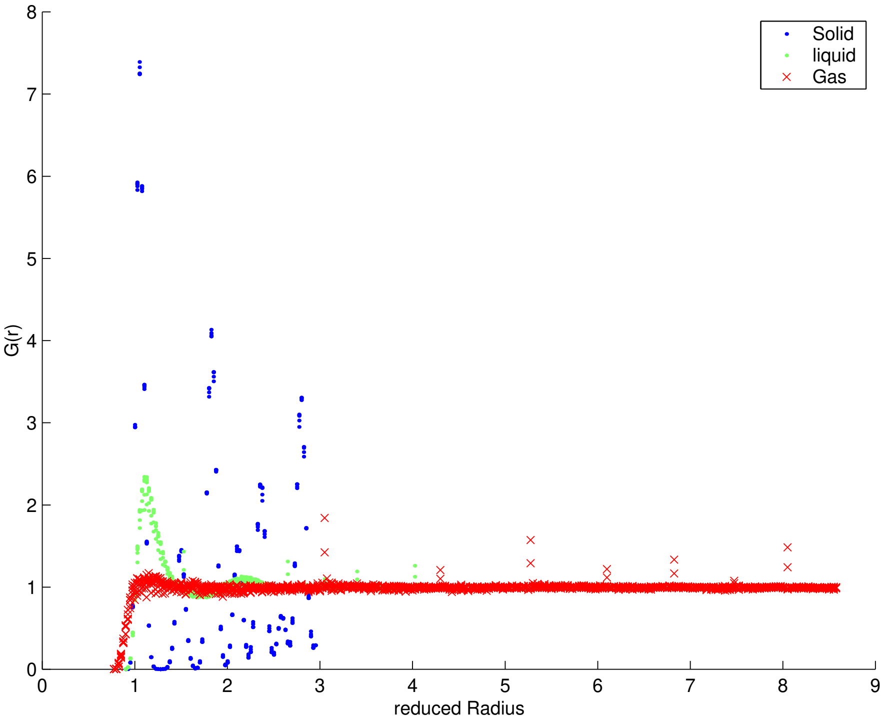

Figure 1: Radial distribution Function

2 Problem 6

We plot out the radial distribution function as fig. 1.

We can see that the peaks of g(r) in solid are quite sharp at certain radius. And the g(r) of gas is nearly disappearing, which means that molecules of gas are moving quite often.And our simulations are under the following 3 condition:

- Solid: TR=0.5, DR=1.2;
- liquid: TR=1.0, DR=0.4
- GAS: TR=9.0, DR=0.05

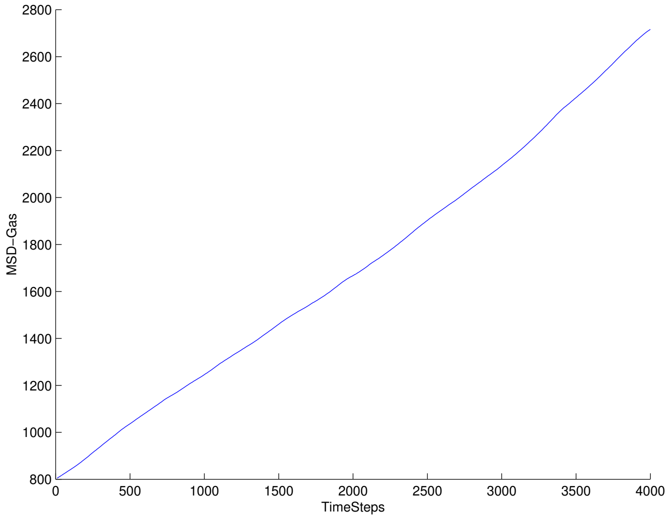

Figure 2: Gas simulation with the condition that TR=9.0,DR=0.05,NEQ=2000,MAXKB= 4000,NP=256

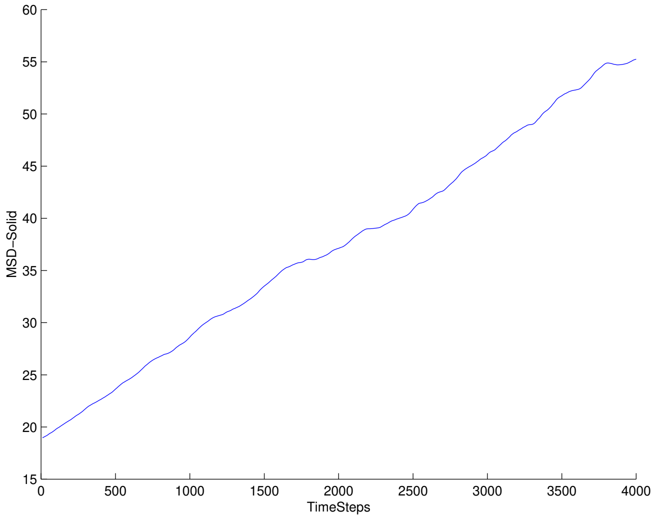

Figure 3: Liquid Simulation with the condition that TR=1.0, DR=0.4, NEQ=2000, MAXKB=4000, NP=256

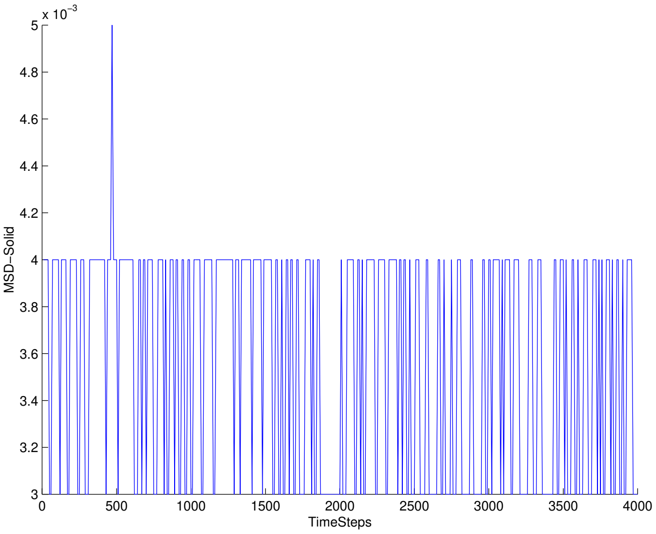

Figure 4: Solid Simulation with the condition that Tr=0.5, DR=1.2, NEQ=2000, MAXKB=4000, NP=256

As the glass system, we run the system until it reaches equilibrium and then quench it by setting the temperature suddenly to zero. Fig.5 and 6 show G(r) and MSD of the system. From fig. 5 spectrum looks different from liquid and solid. The first peak is higher than the liquid . MSD of glass should be increasing but in a very slower rate than liquid as the time goes.

If we decrease the temperature very quickly the process of crystallization will not occur. However if we decrease it slowly, crystallization will occur.

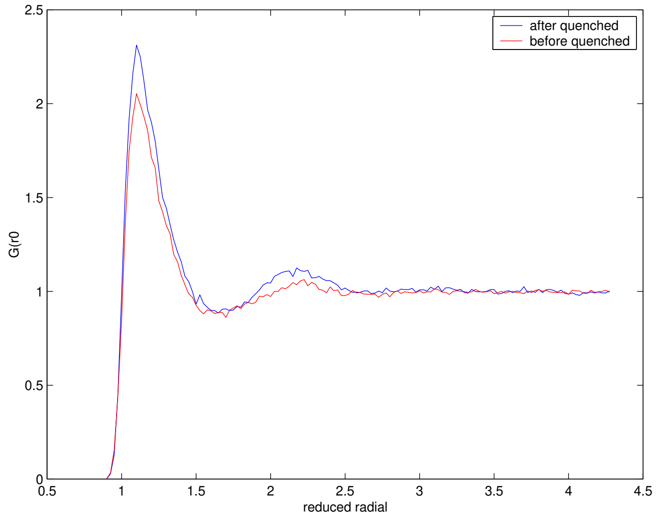

Figure 5: G(R) for glass

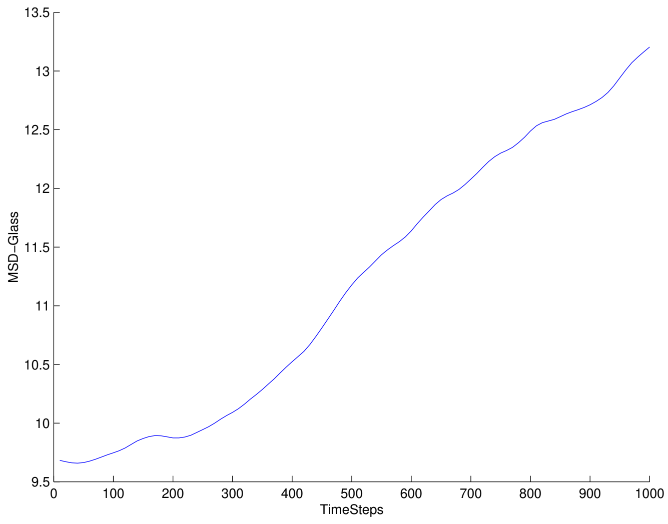

Figure 6: MSD for glass