VISUALIZATION OF NOBLE GAS DIFFUSION USING MOLECULAR DYNAMICS SIMULATION

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Term Project Report for MAE-8001

Submitted By

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Abstract

The proposed study is to learn molecular dynamics (MD) simulation to visualize the behavior and trajectories of atoms/ molecules/ charges in space with respect to different thermophysical quantities. We have used LAMMPS software [1] for our MD simulation. We have built the input script for LAMMPS, and then run the simulation to visualize the diffusion of the atoms. We have conducted the MD simulation of a binary gas and visualized the trajectories and positions of particles at different times.

1. Introduction

Every molecule in space has a tendency to reach lowest energy state. Gaseous molecules have a higher tendency to spread rapidly and diffuse to the whole control volume in order to achieve minimum energy state. Diffusion is a process in which matter moves from a location of high concentration to a region of low concentration due to random mobility of molecules. The applications of diffusions are many in science and engineering. Carbon is diffused into iron to prepare steel. The amount of carbon diffused into iron from the surface determined the hardness and toughness of the steel. Semiconductors are created by doping one material (usually silicon) with a small number of atoms from a different valency material. This is referred to as doping, and it indicates that the material contains an excess of charge carriers (electrons if the valency of the dopant is greater than that of the silicon, or holes if it is less). Diffusion doping involves immersing silicon in a gas containing dopant atoms and heating it to high temperatures. Dopant atoms diffuse into silicon by diffusing down the chemical potential gradient.

Therefore, it is essential to study the diffusion of molecules and ions. The aim of our study is to visualize the diffusion phenomena at molecular level. Molecular dynamics (MD) simulation was used to investigate the diffusion of binary fluid in a 2-D simulation box using LAMMPS software. The fluid (gas) atoms interact with one another via the Lennard-Jones potential. To achieve energy minimization, we visualized the diffusion of gaseous atoms in space.

2. Molecular Dynamics

Molecular dynamics is a computer simulation method that uses a classical approximation to represent chemical systems to examine the physical movements of atoms and molecules, whose phenomena are usually too small to be observed directly. The atoms and molecules are allowed to interact for a set amount of time, revealing the system's dynamic evolution. Researchers can examine the dynamics of complex chemical systems using the simplified representation rather than the quantum mechanical explanation. Atomic and molecular trajectories are derived by computationally solving Newton's equations of motion for a system of interacting particles, where forces between particles and their

potential energies are commonly estimated using interatomic potentials or molecular mechanics force fields. By Newton's equation of motion, the force *F* of the particle is the derivative of interatomic potential *U* with respect to the position *r* of the particles.

$$F = -\frac{dU}{dr} \quad (1)$$

Then, the acceleration *a* of the particle having constant mass *m* can be directly derived by Newton's second law.

$$F = m\,a \quad (2)$$

In short time interval Δt, the acceleration *a* can be considered as constant. The position and velocity of each particle can be directly determined using initial position and acceleration.

$$r = \frac{1}{2}\,a\,\Delta t^2 + V_o \Delta t + r_o \quad (3)$$

$$V = V_o + a\,\Delta t \quad (4)$$

V_o and r_o are initial velocity and position of the particle. MD simulations employ a variety of numerical approaches for determining particles' trajectories.

3. Description of MD simulation operations

For MD simulation, a two-dimensional rectangular container with dimensions (unitless) of 60 by 60 is employed. The simulation is done with simple Lennard-Jones (lj) units. In lj style, all quantities are unitless. Particles (or atoms) are divided into two sorts, each with an atomic mass of one. 150 type-2 atoms are randomly placed inside a 15-radius cylinder, while 1000 type-1 atoms are placed outside the cylinder within the rectangle container. Both sorts of atoms have the same mass of 1. Periodic boundary conditions are applied to the system. Energy minimization operation is initially imposed to the system. A conventional 12/6 Lennard-Jones potential with a length cutoff of 2.5 sigma is indicated by the pair style "lj/cut 2.5." For one or more pairings of atom types, the keyword "pair_coeff" sets the pairwise force field coefficients.

Our first LAMMPS input file reads:NVE

```
# ----------        Initialization
units               lj
dimension           2
atom_style          atomic
pair_style          lj/cut 2.5
boundary            p p p
# ---------- System definition
region              mybox block -30 30 -30 30 -0.5 0.5
```

```
create_box          2 mybox
region              mycylin cylinder z 0 0 15 INF INF side in
region              mycylou cylinder z 0 0 15 INF INF side out
create_atoms        1 random 1000 341341 mycylou
create_atoms        2 random 150 127569 mycylin
# ------------- Simulation settings
mass                1 1
mass                2 1
pair_coeff          1 1 1.0 1.0
pair_coeff          2 2 0.5 3.0
neigh_modify        every 1 delay 5 check yes
dump                mydmp all atom 10 dump.min.lammpstrj
# ------------- Run
thermo              10
minimize            1.0e-4 1.0e-6 1000 10000
write_data          data.min.lammps
```

The simulation settings specify the Lennard-Jones coefficients (i.e., the depth of the potential well ϵ and the distance at which the particle-particle potential energy is zero σ for interactions between atoms of type 1) for interactions between atoms of type 1. The Lennard-Jones coefficients for interactions between type 2 atoms are defined as 0.5 and 0.3. The simulation begins with minimize command that operates the energy minimization. The atoms' coordinates are adjusted until one of the stopping criteria is met in an energy minimization. There are four stopping criteria: (a) the change in energy between two iterations is less than 1.0e-4, (b) The maximum force between two atoms in the system is lower than 1.0e-6, (c) the maximum number of iterations is 1000, the maximum number of times the force and the energy have been evaluated is 10000.

The initial velocity was chosen using the ‘velocity create’ command attributes from a second input script file. The goal of setting initial velocity is to initialized the system with an equal temperature of 1 (unitless).

```
# ------------- Run
velocity    all create 1.0 4928459 mom yes rot yes dist gaussian
fix         mynve all nve
fix         mylgv all langevin 1.0 1.0 0.1 1530917 zero yes
fix         myefn all enforce2d
timestep    0.005
```

```
thermo      50000
run         1500000
```

The additional keywords verify that the system has no linear or angular momentum, and that the resulting velocities are Gaussian in distribution. The langevin thermostat's 'zero yes' keyword ensures that the total random force is zero. The first fix updates the locations and velocities of the atoms in the group 'all' using constant NVE integration [micro-canonical ensemble with constant number of atoms (N), constant volume (V), and constant energy (E)]. The second fix uses a Langevin thermostat to control the temperature of the atoms in group 'all,' with a desired temperature of 1 and a damping parameter of 0.1. The third fix makes sure the atoms stay in the 2D enclosure. Finally, we select a timestep and instruct LAMMPS to print information in the terminal every 50000 timesteps.

4. Results and discussions

Initially there is only type-2 atoms were inside the cylinder. We have applied MD simulation to a binary fluid system and applied energy minimization operation in order to uniformly distribute the particles in two separate regimes. The initial equilibrium position of particles is represented in Figure 1. The green color corresponding to the particles of type-2 and red represents the type-1.

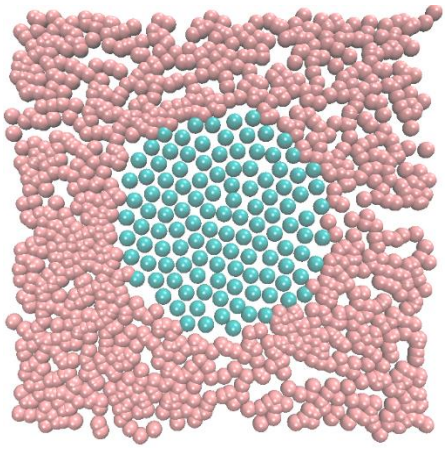
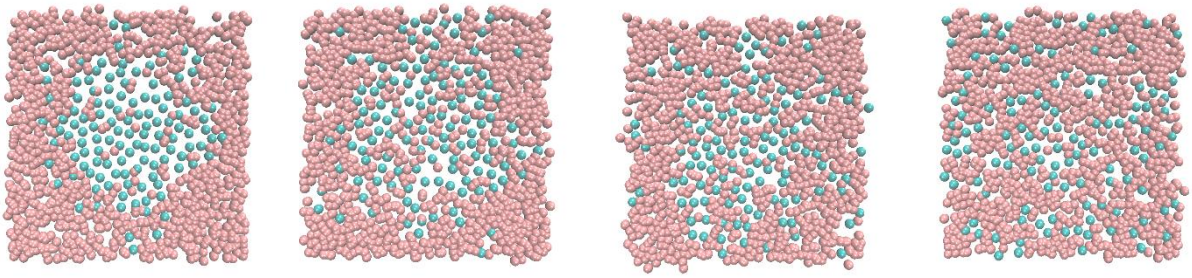


Figure 1. Initial position of LJ particles.

After the equilibrium is achieved, a velocity is applied to initialize the system with constant temperature. Then NVE micro-canonical ensemble is performed. The timestep used to run the simulation is 0.005 pico-second for 1,500,000 steps (7500 ps). The particles started to move and interact with one another. Particles of both types cross their initial position and rearrange themselves into new equilibrium positions.



500 ps 1500 ps 2500 ps 7500 ps

Figure 2. Position of particles at different time.

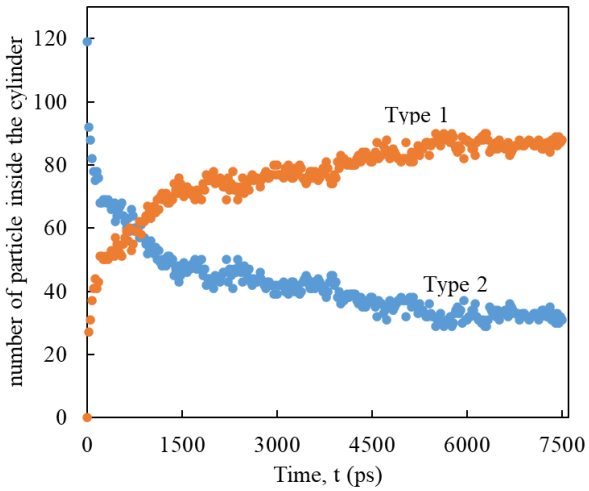


Figure 3. Number of particles of type-1 and type-2 after

Figure 3 shows that there are no type-1 particles inside the cylinder at first (circular regime). However, as time passes, the number of type-1 particles inside the cylinder has increased, as has the number of type-2 particles outside the cylinder.

5. Conclusion

The sole purpose of this study is to learn molecular dynamics simulation using LAMMPS. We have visualized the diffusion phenomena of binary gas from molecular level. The particles become excited and interact with one another vigorously while the temperature of the system is increased. We have visualized that initially the particles or type-2 were only inside the cylinder, whereas type-1 were outside the cylinder. However, with time, they begin to shift from a higher to a lower concentration regime in the diffusion process. We will further study the diffusion of noble gas inside porous media or metal surface.

6. References

[1] https://www.lammps.org/