# 1 Introduction

In this assignment, I simulate a gas container with $size = 30 * 30$ using velocity-verlet ODE algorithm.

# 2 Velocity-Verlet Algorithm

$$x_{n+1} = x_n + v_n h - \frac{1}{2} x_n h^2 \tag{1}$$

$$v_{n+1} = v_n - \frac{1}{2}(x_n + x_{n+1})h \tag{2}$$

# 3 Molecular Dynamics

Assume a gas container that at first all of particles are in the left part of it. After a while, it will spread in the container.

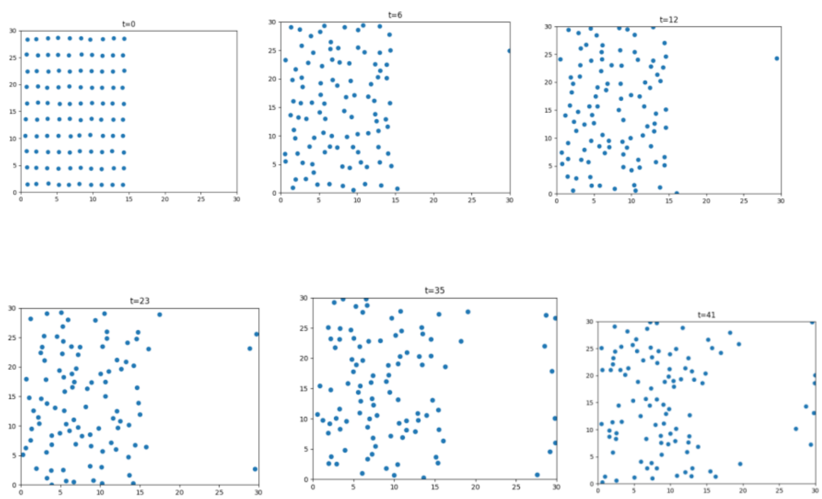


Figure 1: evolution of our gas container, the initial configuration is a simple cubic lattice on the left side of the container.

# 4 Equilibrium

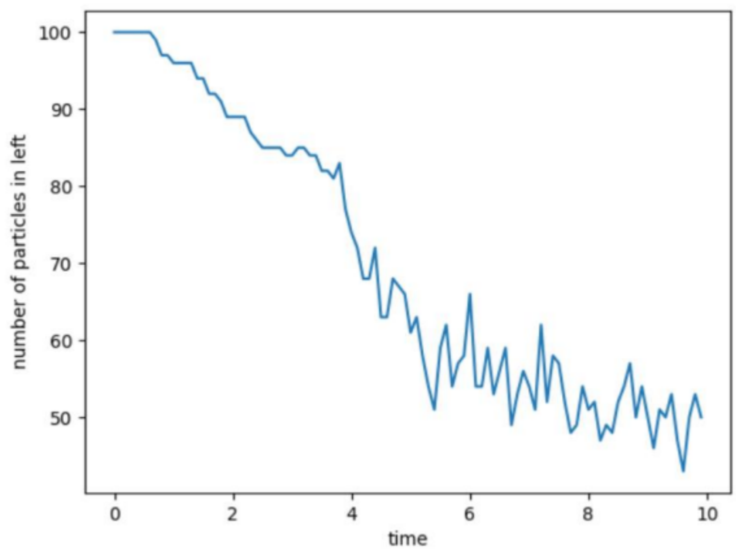


Figure 2: The ratio of the particles on the left side of the container to the total number of particles starts out equal to 1.0.

# 5 Conservation of Energy

In this section, I show the conservation of energy. For calculating the potential energy, Lennard-Jones Potential is used:

$$V_{LJ} = 4\epsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}] \tag{3}$$

where r is the distance between each of two particles which reinforced each other. For kinetic energy we have:

$$K = \sum_i \frac{1}{2} v_i^2 \tag{4}$$

# 6 Van der Waals Equation

$$(P + a\frac{n^2}{v^2})(V - nb) = nRT \tag{5}$$

Where P and V are pressure and volume respectively, and a and b are constants. It could be calculated that

$$P = \frac{1}{V/N - b^*} T - \frac{N^2}{V^2} a^* \tag{6}$$

In this section, Van der Waals Equation is simulated and P-T graph is shown. For our gas $a^* = 2.26$ and $b^* = 1.37$.